1 OPUS Basics

This chapter contains basic information about the most important OPUS features and provides useful notes on how to work with the OPUS tools.

1.1 Basic Software Features

Browser	Contains the name and directory path of the spectrum file currently loaded. For further details refer to chapter 1.11.
Dialog box	The OPUS dialog boxes consist of different tabs. Click on these tabs to change between them. Buttons and drop-down lists are only enabled, if they are displayed in black. Grayed buttons or other items are disabled.
Drag & Drop	OPUS supports drag & drop, a method to move graphical elements by using the mouse. You can drag single elements of a graphical user interface from one particular position and drop them at a different position. Drag & drop simplifies e.g. the *Copy* and *Paste* process of files. In this case you have to select the file first, press the left mouse button while moving the file to the respective dialog box (or window). If you release the mouse button, the file will automatically be loaded into the dialog box (or window) selected. Double clicking on the spectra file name allows to move spectra files to a specific dialog.
Pop-up menu	There are several pop-up menus in OPUS available. To display a pop-up menu right click anywhere in a window.
Shortcut	OPUS supports shortcuts (a key or set of keys that performs a pre-defined function), e.g. copy (*Ctrl+C*), cut (*Ctrl+X*) and paste (*Ctrl+V*). To use these shortcuts, you first have to select the text or file you want to process.
Single-click mode	A single click on an icon in the toolbar or wizard performs the command selected based on the parameters last set. In some cases the single click opens the setup dialog before performing the command.
Toolbars	OPUS provides toolbars which can be individually configured to quickly access frequently-used functions. By default, the OPUS interface contains one single toolbar. For further details on toolbars refer to chapter 1.8 and 3.12.5.
Tooltips	Next to each icon context-sensitive tooltips pop up when you position the cursor on that icon.
Wizard	The OPUS wizard is an interactive help tool that suggests a series of OPUS commands to perform a particular application. For further details refer to chapter 1.12.

1.2   Starting OPUS

Click on the OPUS program icon on the Windows start menu. The icon is automatically displayed if the OPUS installation has been completed successfully.
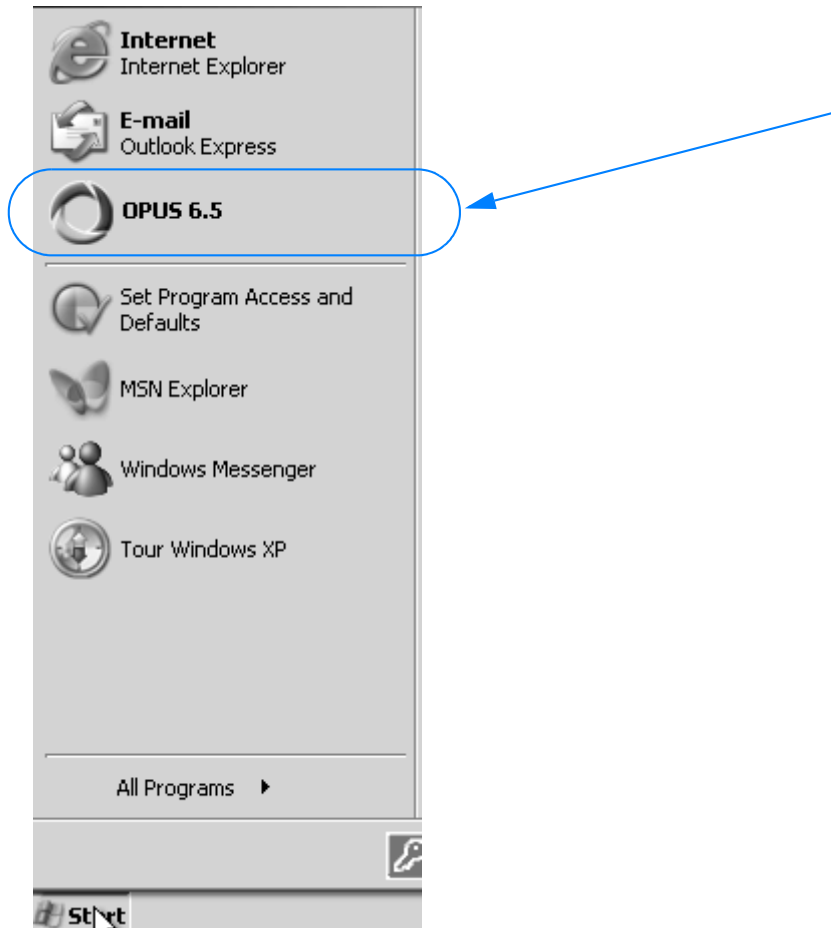

Figure 1: Windows start menu

Setting OPUS language

OPUS is available in several different languages. To change the language originally installed proceed as follows:

1   Click on the Windows *Start* button and right click on the OPUS icon.

2   Select the *Properties* command from the pop-up menu. The following dialog opens:
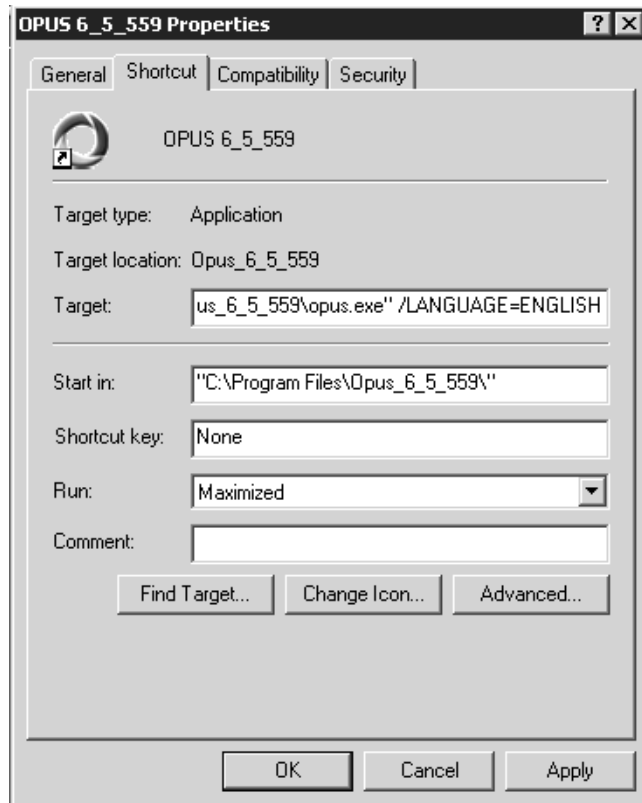
Figure 2: Properties dialog

Depending on your Windows version this dialog may look slightly different.

3 Add the correct language parameter into the *Target* entry field on the *Shortcut* tab. **Make sure that you type the parameter in capital letters.** If the parameter is not recognized, OPUS will use the default language, i.e. English. The following parameters are possible:

- *OPUS/LANGUAGE=CHINESE* (starts OPUS in Chinese)
- *OPUS/LANGUAGE=ENGLISH* (starts OPUS in English)
- *OPUS/LANGUAGE=FRENCH* (starts OPUS in French)
- *OPUS/LANGUAGE=GERMAN* (starts OPUS in German)
- *OPUS/LANGUAGE=JAPANESE* (starts OPUS in Japanese)
- *OPUS/LANGUAGE=SPANISH* (starts OPUS in Spanish)

4 To confirm the setting click on the *OK* button.

Note: The language setting will be transferred to OPUS as parameter when starting the program next time.
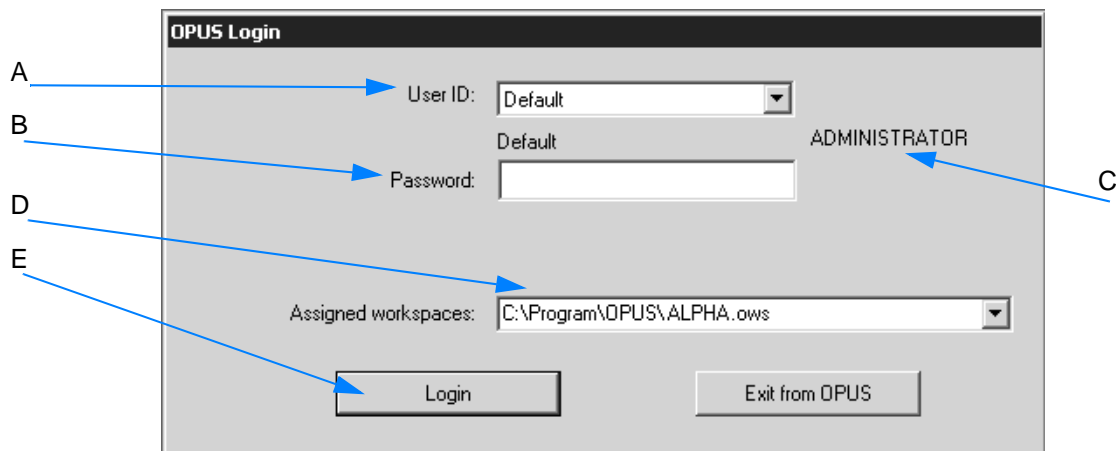
1.3   Login

Figure 3: OPUS Login

A Select your *User ID* from the drop-down list. OPUS provides an independent user account system which regulates the access. **If you use OPUS for the very first time, the *User ID* drop-down list includes the two pre-defined user records *Default* and *Administrator*. Select either one of them.**

B Enter *OPUS* into the *Password* entry field. The password is case sensitive. Once you have assigned yourself a user record in OPUS, it is possible to determine your own *User ID* and *Password*.

C OPUS includes different accounts for operator and administrator rights. Users defined as *Operator* have limited access rights compared to users defined as *Administrator*. The rights depend on the *User ID* selected.

D The *Assigned workspaces* identify the user interface and access right. You can always select those workspaces from the drop-down list which have been defined for your *User ID*. When you use OPUS for the first time, we recommend not to change the standard *ALPHA.ows* or *Default.ows* workspace.

E Click on the *Login* button to open the *About OPUS* window.
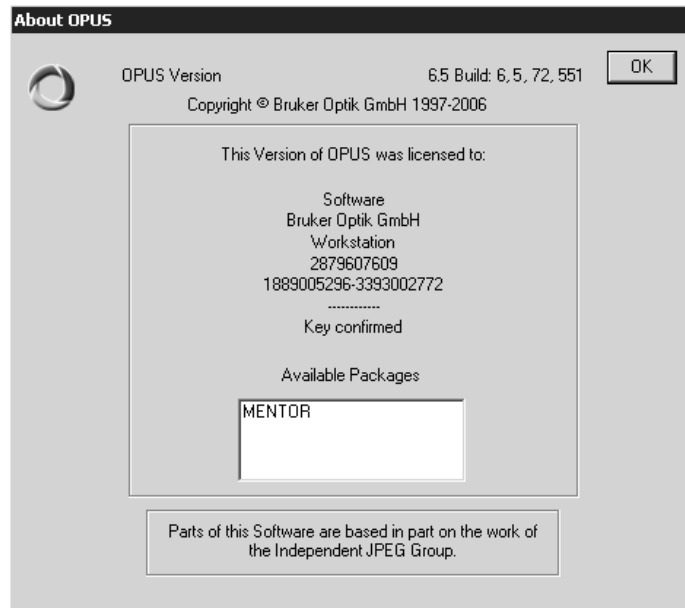
Figure 4: About OPUS

It shows the serial number of your OPUS copy and the registered user name as well as the name of the basic OPUS software package registered.

Click on the *OK* button to open the OPUS user interface.

1.4   Automatic Test Procedure

As soon as you have opened OPUS, OPUS and ALPHA begin to communicate with each other and OPUS starts automatically a performance test. In the lower right corner of the OPUS interface, a yellow message bubble appears informing you that the performance test is running.

After the test has been completed successfully, the status light turns green and the *Accessory Test* dialog window opens. See the following figure:
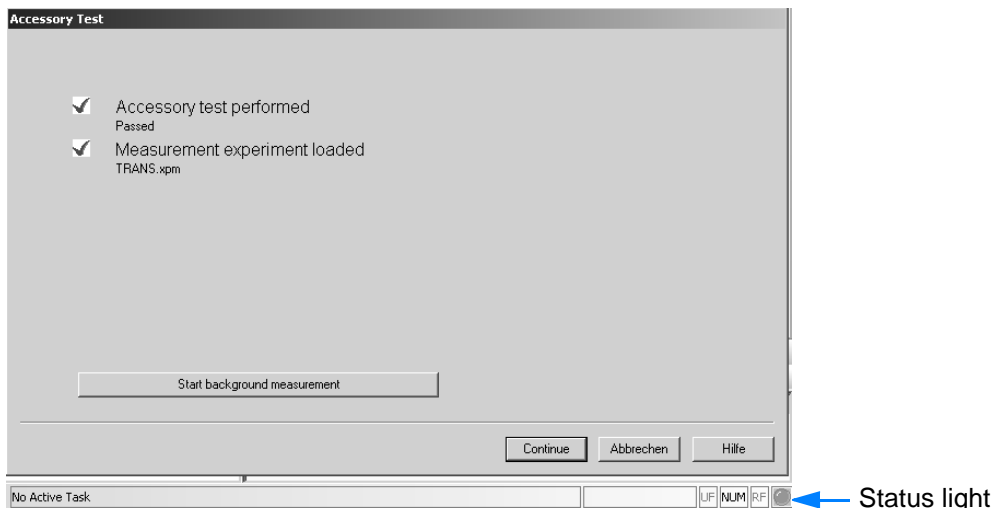
Figure 5: Message of a passed accessory test

Now you can either close this dialog by clicking on the *Continue* button or start a background measurement.

Note: If the accessory test has failed, see chapter 10. In addition, the OVP - PQ Test Protocol opens in form of a pdf file. This pdf file is stored automatically under *OPUS path\Validation\Reports.*

Differences between Performance Test and Instrument Test

Both tests check whether the spectrometer achieves the specified performance. But they differ in the following aspects:

	Performance Test	Instrument Test
The test procedure includes the following tests	• Signal-to-noise test • Deviation from 100% line	• Signal-to-noise test • Deviation from 100% line • Wavenumber accuracy test
Number of test measurements	1	11
Test duration	about 1 minute	about 5 minutes
When is the test performed?	• automatically after OPUS has been opened again • automatically after ALPHA has been accessed again • automatically after the measurement module has been substituted by another measurement module	• automatically when the PC and ALPHA communicate with each other for the very first time (see also the *Installation Manual*.) • manually (i.e. you have to start the instrument test yourself) after the defined instrument test validity period has expired **Note: The factory-set validity period is 7 days.**

See also chapter 10.3.3, 10.3.4 and 10.3.5.

1.5   Workspace

OPUS uses the following default workspaces which are identical:

- ALPHA.ows
- Default. ows

The following settings are stored in the OPUS workspace:

- User rights
- Configuration of toolbars and windows
- Parameter settings of all commands
- Configuration of menus and pop-up menu
- User name and password

To modify the workspace or create a new one you need the right to do so. This is set by means of the *User Settings* command in the *Setup* menu. Activate the respective check boxes on the *Rights* tab.
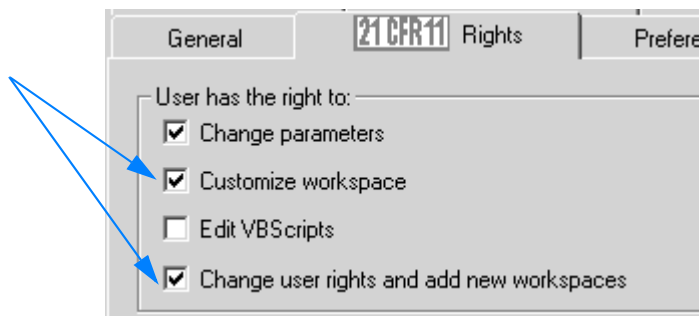
Figure 6: User workspace right

> **Note: If you have modified the workspace, e.g. by re-positioning toolbars, these changes will automatically be stored when you exit OPUS.**
>
> **If you have created a new workspace, a dialog pops up requesting the name of this new workspace when you exit OPUS.**

For further information on this subject refer to chapter 3.12.7.

1.6   Access Control

OPUS has an access control mechanism which is shown in the chart below:
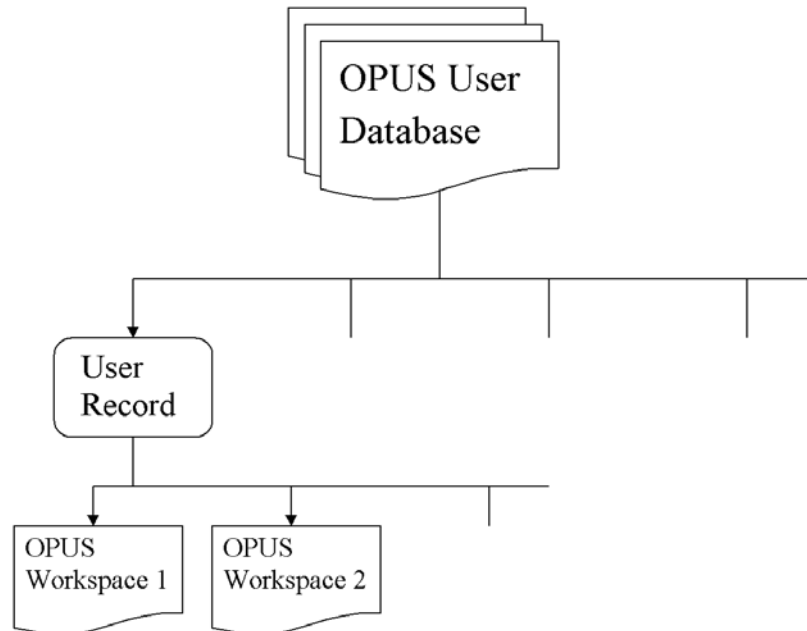
Figure 7: OPUS access control chart

The *OPUS User Database* includes all *User Records*.

The *User Records* comprise:

- User ID
- Password
- Operator Name
- User Group (Administrator, Operator)
- Accessible Workspaces

The *Workspaces* comprise:

- Menu Contents
- Toolbar Contents
- Access Rights within OPUS
- Other Settings (e.g. file increment mode, display limits)

1.7   User Rights

OPUS distinguishes between three different types of users:

- Administrator
- Lab Manager
- Operator

The different user groups have the following rights in OPUS:

User Group	Workspaces	User Settings
Administrator	• Access to all • Right to modify all • Right to create new ones	• Complete access • Right to change them
Lab Manager	• Access to all • Right to modify all • Right to create new ones	• No access
Operator	• Access to the one(s) assigned	• No access

The user rights are defined by the *User settings* command in the OPUS *Setup* menu (see chapter 3.12). The *Administrator* has to ensure that the *Operator* has only access to special commands within the OPUS workspace assigned to the *Operator*.

1.8   Interface

The interface appearance depends on the screen settings and operating system used. Thus, the screen display of the following dialog boxes may not show exactly the screen contents displayed on your screen.

BRUKER recommends a minimum graphic resolution of 800 x 600 pixel and *True Color*.
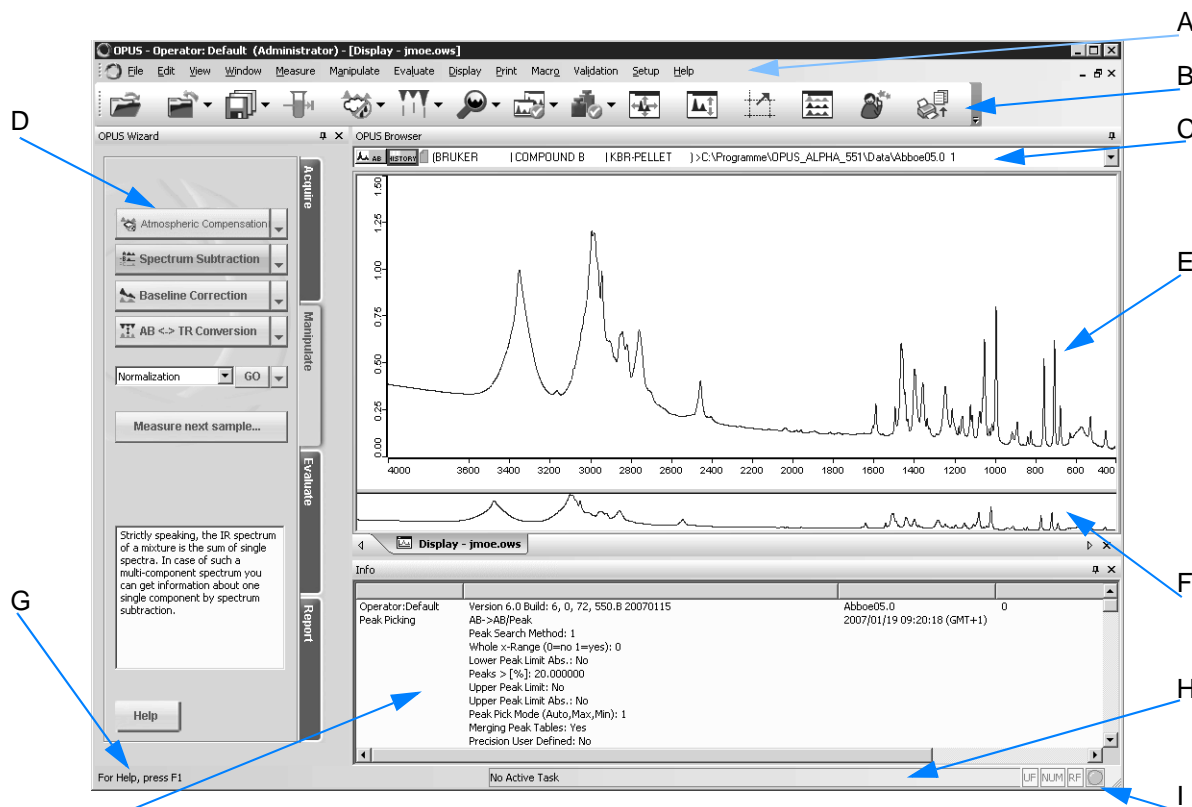
Figure 8: OPUS user interface

A Pull-down menus

B Toolbars

C Browser

D Wizard

E Spectrum window

F Overview window

G Context-sensitive online help

H Status bar (indicating background tasks)

I   Instrument status

J Information view

How does OPUS indicate different views?

The OPUS views which you work with are indicated by tabs. Each tab has a different color to be able to distinguish between the views.
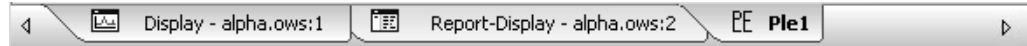
Figure 9: Tabs of different OPUS views

1　Click on these tabs to change from one view to the other. The frame around each view has the same color as the corresponding tab.

2　If several views are open simultaneously, use the ◀ ▶ on the left and right to change between the different views.

How to configure menus and toolbars?

1　Select the *Customize Menus* or *Customize Toolbars* command from the *Setup* menu.

2　Click on the *Toolbars* or *Menu* tab.

3　Specify the settings. For detailed information refer to chapter 3.12.5 or 3.12.6.

4　Restart OPUS to activate the settings made.

Note: The tool bar configurations are stored together with the workspace settings in one file. This file has the extension *.ows. OPUS default settings are stored in the DEFAULT.OWS workspace. For details on workspaces, see chapter 1.5.

1.9 Icons

Icons facilitate working with OPUS and are part of the toolbars and menus. Depending on the command selected the following actions can be produced when clicking on an icon.

Icon	A single click...	Allows...
	...on the icon	...to open the command dialog ...to execute the command
	...on the icon	...to execute the command
	...on the triangle	... to open the - command dialog - method setup dialog - interactive view - online help

The following table includes all icons available for the OPUS Mentor software package. For detailed information on the single OPUS commands refer to chapter 3.

Menu	Icon	Definition	Menu	Icon	Definition
File		Load File	Edit		Edit Parameter
		Unload File			Replay
		Unload All Files			Cut
		Save File As			Copy
		Undo Changes			Paste
		Save File			
		Send File			
		Clone Entry			
		Clone Original			
		LabJournal			

Menu	Icon	Definition	Menu	Icon	Definition
		Open			
Window		New Spectrum Window	Measure		Setup Measurement Parameters
		New Report Window			Measurement
		Cascade			Cleanness Test Setup
		Tile			Cleanliness Test
Manipulate		Baseline Correction	Evaluate		Integration
		Spectrum Subtraction			QUANT Builder
		AB <-> TR Conversion			Quantitative Analysis
Manipulate		Spectrum Calculator	Evaluate		Signal-To-Noise Ratio
		Cut			Peak Picking
		Straight Line Generation			Quick Compare Setup
		Normalization			Quick Compare
		Convert Spectra			Spectrum Search
		Smooth			Initialize Library
		Derivative			Store Spectrum in Library
		Atmospheric Compensation			Library Editor
					Band Assignment Chart
Display		Back	Print		Print Spectra
		Forward			Quick Print
		Stacked			Print

Menu	Icon	Definition	Menu	Icon	Definition
		Scale All			
		Scale Y			
		Page Back			
		Page Forward			
		Zoom In			
Macro		New Procedure	Validation		Setup instrument test
		Edit Procedure			Run instrument test
		Execute Procedure			Optic Configuration, Service
Setup		User Management	Help		FT-IR Tutorial
		Change User Password			About OPUS
		New Workspace			
		Close Workspace			
		Send Workspace			

1.10 Data Blocks

OPUS spectrum files can contain different kinds of spectra, evaluation results or reports. This kind of data is depicted in data blocks in the OPUS browser.

The following table includes all data blocks available for the OPUS Mentor software package.

Data block	Abbreviation	Definition
	AB	Absorptions spectrum
	ABARI	Arithmetical result (absorbance)

Data block	Abbreviation	Definition
TRARI	TRARI	Arithmetical result (transmittance)
ANNO	ANNO	Annotation
ATR	ATR	ATR spectrum
1DER	1DER	First derivative
2DER	2DER	Second derivative
nDER	nDER	n th derivative
GEN.REP	GEN.REP	General report
HISTORY	HISTORY	Protocol
IFG	IFG	Interferogram
RIFG	RIFG	Reference interferogram
SIFG	SIFG	Sample interferogram
INFO	INFO	Information block
INTEG	INTEG	Integration report
KM	KM	Kubelka-Munk spectrum
METHOD	METHOD	Method
PEAKS	PEAKS	Peak table
RPH	RPH	Reference phase spectrum
SPH	SPH	Sample phase spectrum
RPOW	RPOW	Reference power spectrum
SPOW	SPOW	Sample power spectrum
QC	QC	Quick Compare
QTEST	QTEST	Quality test
QUANT	QUANT	QUANT report
REFL	REFL	Reflectance spectrum
LREFL	LREFL	Logarithm of reflectance
REPORT	REPORT	Report
RSC	RSC	Single-channel spectrum, reference
SSC	SSC	Single-channel spectrum, sample
SEARCH	SEARCH	Search result
STR	STR	Molecular structure
SUBTR.	SUBTR.	Subtraction report
TR	TR	Transmittance spectrum

Data block	Abbreviation	Definition
...	...	Unknown data block
???	???	Unknown data block
?	?	Unknown spectrum type

1.11   Browser

The OPUS browser shows the spectrum files together with the corresponding data blocks.

Note: If the browser is not displayed, make sure that the *Browser* option is checked in the *View* menu.

By default, the browser is displayed above the spectrum window.
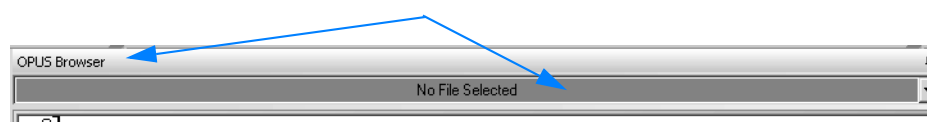
Figure 10: Browser displayed in OPUS

When loading a spectrum file...

...it is displayed in the OPUS browser as follows:
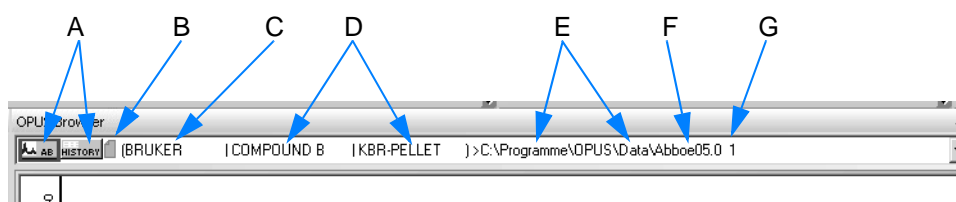
Figure 11: Browser as drop-down list

A Data blocks
Each spectrum file can contain different types of data blocks (see also chapter 1.10). To select a data block left click on the particular block. A red frame around the data block indicates that this data block has been selected. The number of data blocks to be displayed can be globally set up, see chapter 3.12.7.

B Status of spectrum file
A spectrum file can have one of the following types of status:
• light blue: file has not yet been edited, i.e. the original parameter settings are still available
• red: file has been edited, i.e. specific parameters have been changed

C Company name

D Sample type

E Data path of spectrum file

F Name of spectrum file

G Number of copies made from the spectrum file
If you have loaded the same spectrum file several times, the copies will be incremented.

When loading several spectrum files...

...only one spectrum file is displayed in the browser, by default. To be able to see all files loaded you have to click on the arrow (on the right side of the browser.
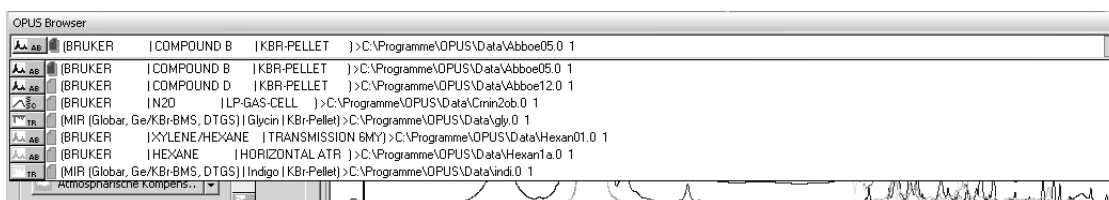
Figure 12: Browser with loaded spectrum files

1.11.1 Hide automatically

The icon allows to automatically hide the browser. In this case the browser is displayed as a blue bar below the toolbar on the left side.

Figure 13: Hidden browser

To unhide the browser...

...position the cursor onto the blue bar below the toolbar. Now, the icon points to the right. As soon as you move the cursor outside the browser on the OPUS interface, the browser will be hidden again.

To have the browser permanently displayed again...

...click on the ⊟ icon as soon as you unhide the browser. To close the browser click on the ✕ icon

1.11.2 Pop-up menus

Two different types of pop-up menus can be generated in the browser:

- pop-up menu to edit spectrum data
- pop-up menu to change spectrum display

To edit spectrum data you open the pop-up menu...

...by right clicking on the <u>name</u> of the spectrum file. The pop-up menu contains the following options:
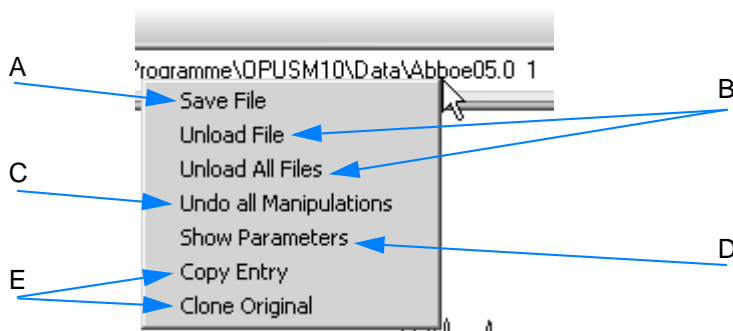
Figure 14: Pop-up menu to edit spectrum data

A Changes made in a file are not automatically saved in the file directory. Therefore, store these changes by using the *Save File* command.

B The file is removed from the spectrum window, but is still available in the file directory.

C Changes made in a file can be undone to restore the original spectrum file.

D All pieces of information on data acquisition of a particular spectrum file can be displayed.

E Both commands allow duplicating spectrum files. The difference between these two commands is that *Copy Entry* copies a data file which has been edited. The *Clone Original* command copies the original spectrum file.

To change the spectrum display you open the pop-up menu...

...by right clicking on a data block of the spectrum file. For further details on this menu refer to chapter 1.13.1.

1.12   Wizard

The wizard is an interactive help tool to measure and edit spectra. Certain OPUS commands are available which allow to manipulate or evaluate spectra. These commands are either available as buttons, this concerns the most frequently and recently used ones, or they are listed in a drop-down list.

Note: If the wizard is not displayed, make sure that the *Wizard Bar* option is checked in the *View* menu.

By default, the wizard is displayed on the left side of the OPUS interface.
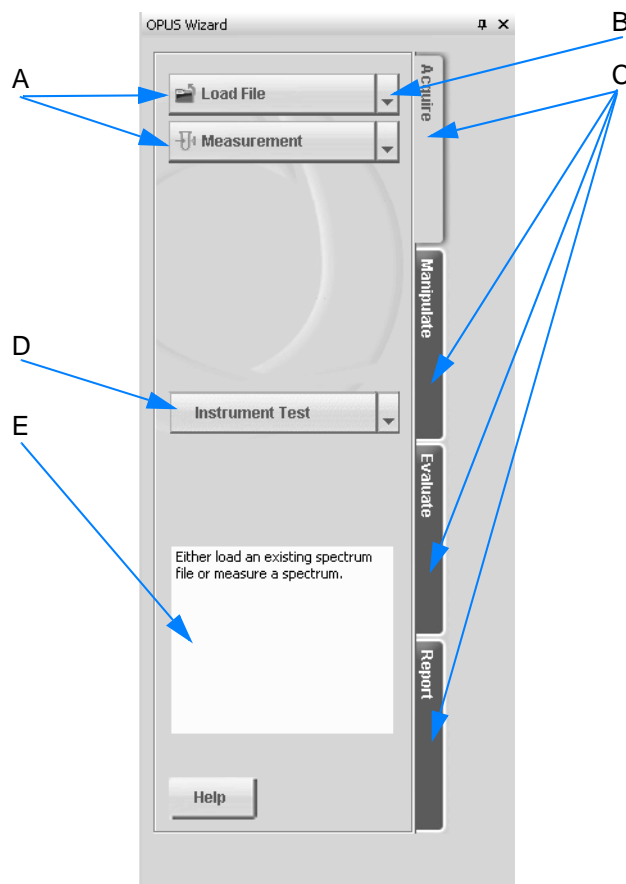
Figure 15: OPUS Wizard

A The wizard contains a series of OPUS commands which can be generally performed by a single click on the respective button.

B If you click on the triangle, an additional menu pops up.

Use this menu to open the setup dialog for the command selected as well as the online help.

C Up to 4 levels are available to edit spectra data.

D An instrument test to qualify the spectrometer performance for daily routine work can be performed.

E This window contains a brief description of the OPUS command currently selected.

1.12.1 Make invisible

The ⊓ icon allows to make the wizard invisible. If you click on this icon, the wizard is hidden in a blue bar below the toolbar.
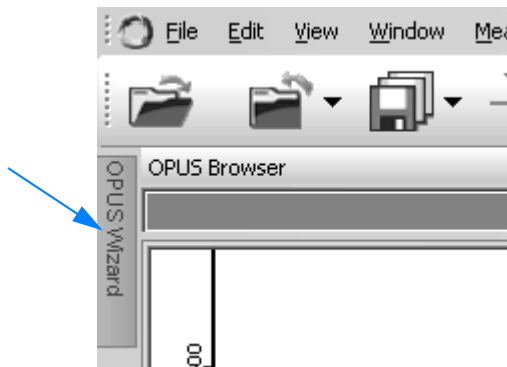
Figure 16: Invisible wizard

To make the wizard visible again...

...position the cursor on the blue bar below the toolbar. The ⊞ icon now points to the right. As soon as you move the cursor outside the wizard on the OPUS interface, the wizard will be hidden again.

To have the wizard permanently displayed again...

...click on the ⊡ icon as soon as the wizard is made visible. To close the wizard click on the ✕ icon.

1.12.2 Levels

Specific OPUS commands are available as buttons on the different wizard levels (B in figure 15). Once you have performed one command you will automatically come to the next possible, and in this particular context, reasonable level. To perform the single commands just click on the respective button.

Acquire
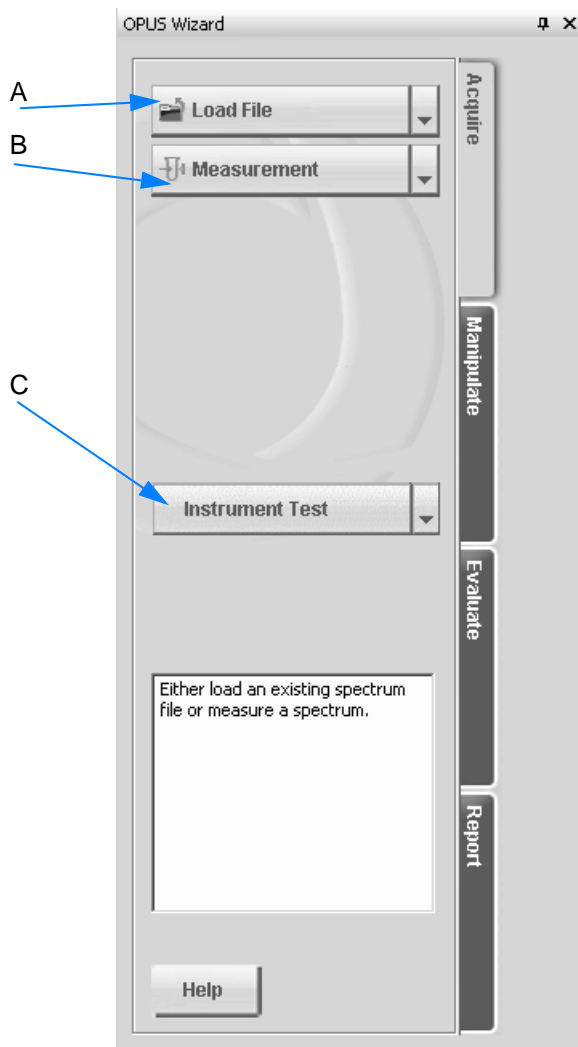
Figure 17: Wizard - Acquire

A On the first wizard level you either load a spectrum or...

B ...perform a measurement.

C It is recommended to perform an instrument test for the current test channel within a specified period of time. Click on the *Instrument Test* button. For detailed information refer to chapter 3.11.

Manipulate

On the second wizard level you edit the spectrum file.
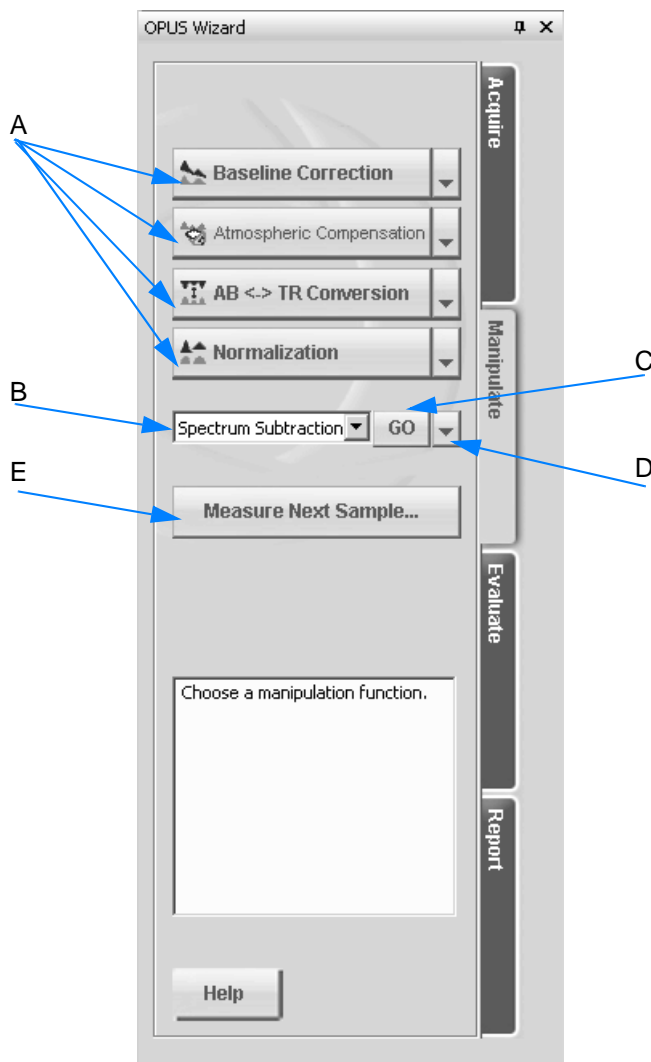
Figure 18: Wizard - Manipulate

A The last 4 manipulation commands previously used are displayed as buttons. If you select a different manipulation command from the drop-down list (B), this command will be displayed as button the next time you start OPUS.

B The drop-down list contains additional manipulation commands.

C Click on this button to start one of the manipulation commands selected from the drop-down list.

D Click on the triangle to open the respective dialog or the online help of the command selected from the drop-down list.

E Start the next sample measurement. The *Measurement* dialog will be displayed.

Evaluate

On the third wizard level you evaluate the spectrum file.
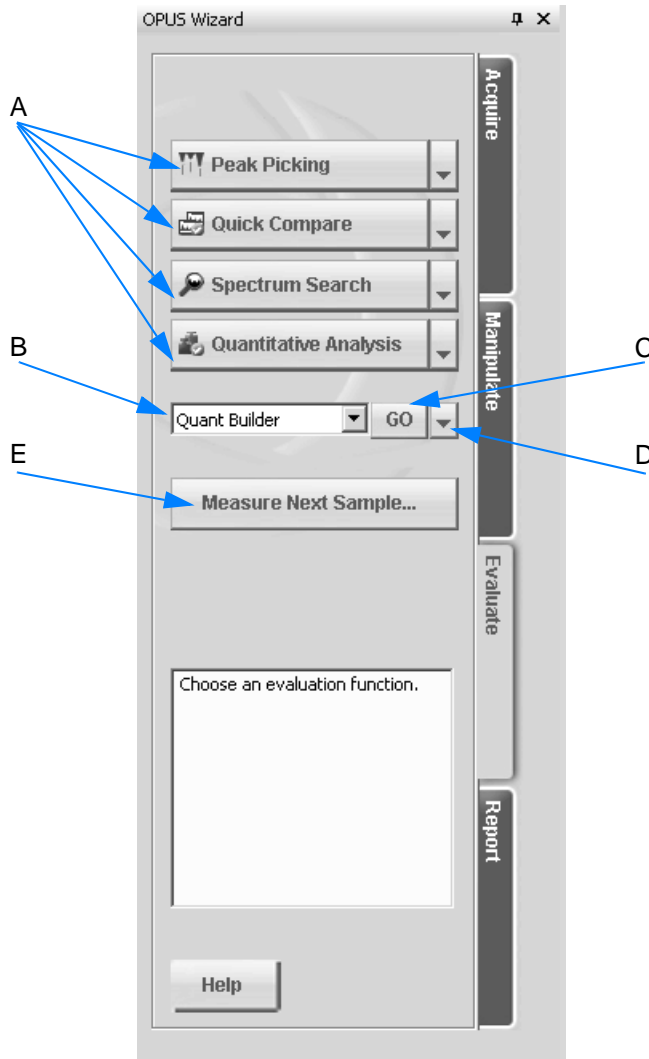
Figure 19: Wizard - Evaluate

A The last 4 evaluation commands previously used are displayed as buttons. If you select a different evaluation command from the drop-down list (B), this command will be displayed as a button the next time you start OPUS.

B The drop-down list contains additional evaluation commands.

C Click on this button to start one of the evaluation commands selected from the drop-down list.

D Click on the triangle to open the respective dialog or the online help of the command selected from the drop-down list.

E Start the next sample measurement. The *Measurement* dialog will be displayed.

Report
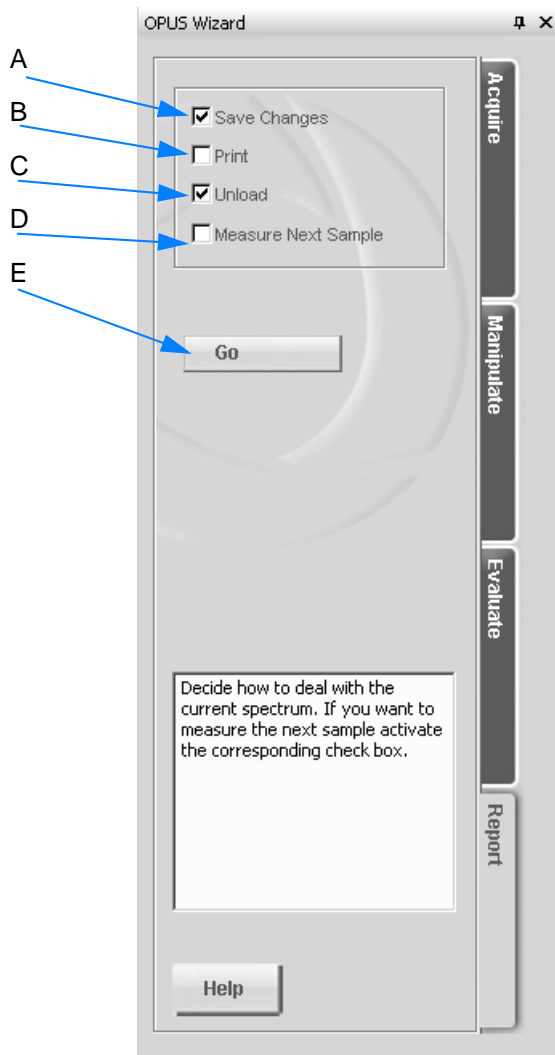
Figure 20: Wizard - Report

A Activate the check box to store the spectrum file, and note the following:

- If you load a spectrum file (by means of the wizard) from a particular directory, this file will automatically be stored into this directory.
- If you measure a spectrum by means of the wizard, this spectrum will be stored into the *C:\Program\OPUS\meas*.** directory. This directory is generated <u>after</u> a measurement has been performed.

B Activate the check box to print the spectrum file.

C Activate the check box to unload the spectrum file, i.e. to remove the spectrum from the spectrum window.

D Activate the check box to measure another sample.

E Click on the *Go* button, to perform the options selected between A - D.

1.13   Spectrum Window

The spectrum window displays either the spectrum of a loaded spectrum file, or the spectrum generated by a measurement.

Note: The default settings for the spectral range are from 4,000 to 400 wavenumbers and from 0 to 1.5 extinction units.
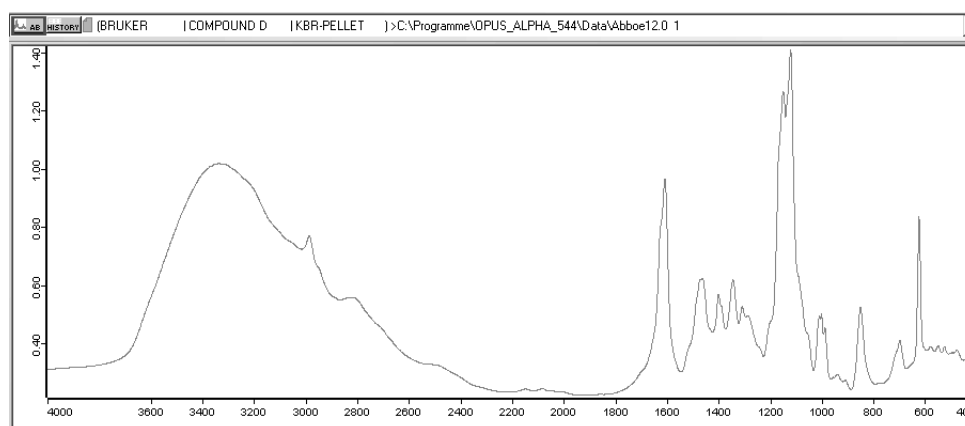
Figure 21: Spectrum window

To scale the spectrum to the complete data range...

...select the *Scale all* command from the *Display* menu. If a file consists of more than one data block, only the first data block is displayed in the spectrum window.

To select a particular spectrum range...

1   ...right click into the spectrum window.

2   Select the *Zoom* → *Zoom In* or *Zoom Out* option from the pop-up menu.

3   Draw a frame around the spectrum range by using the left mouse button.

4   Click on the left mouse button to position this frame.

5   Click on the left mouse button again to have the particular spectrum range displayed in the spectrum window.
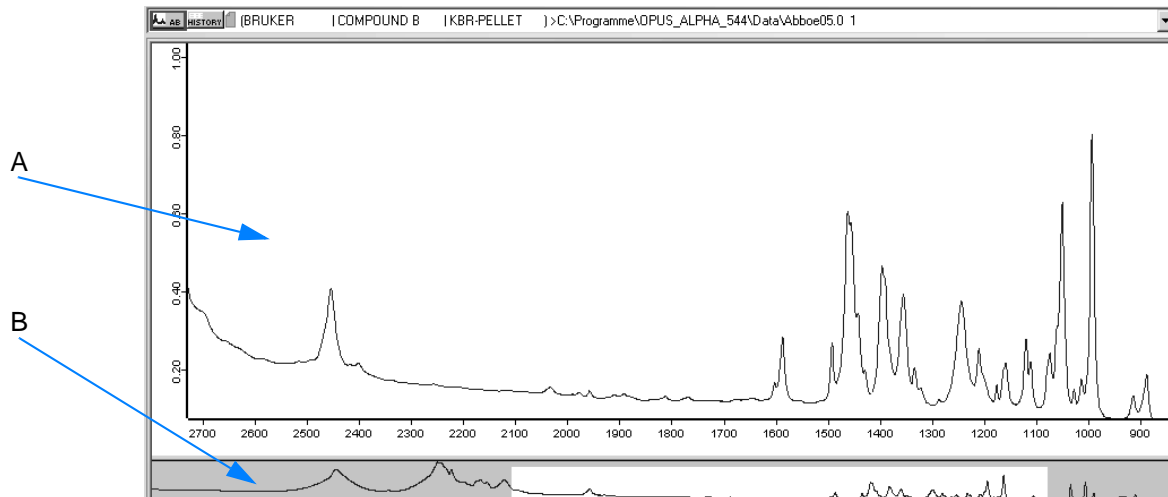
Figure 22: Spectrum range selected

A The spectrum window shows the particular spectrum range selected.

B The overview window shows the complete spectrum range. Note the following:

  • The spectrum range depicted on the white background is exactly the one displayed in the spectrum window.

  • The gray area shows the remaining spectrum.

  If you position the cursor on the white area, the cursor will change from ⬉ to ✥. Now, you can move the borders of the spectral range (white) by pressing the left mouse button.

To enlarge or reduce the spectrum window...

...position the cursor exactly between overview and spectrum window. The cursor changes to ⬍. This allows to re-size the window.

To permanently fix the size of the spectrum window...

...right click between spectrum window and overview window. The *Lock* button is displayed:

If you click on this button, the size of the spectrum window will be fixed and can no longer be changed.

To undo this kind of setting right click between spectrum window and overview window. The *Unlock* button is displayed:

Unlock

When working with several spectrum files simultaneously...

...activate the *Replace in current window* option button in the Settings menu on the *On New File* tab. In this case the window currently loaded will not only be displayed in the spectrum window but also in the browser (see chapter 3.12.7).

1.13.1 Pop-up menu

Right clicking on a spectrum within the spectrum window pops up the following menu.
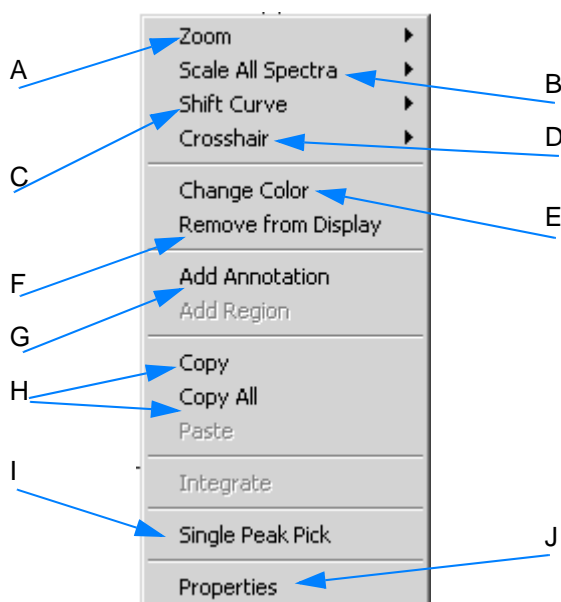
Figure 23: Pop-up menu to change spectrum display

A The spectral range can be enlarged and reduced.

To enlarge part of the spectral range...

- ...select the *Zoom* → *Zoom In* command. A crosshair is displayed in the spectrum window.
- Click on the left mouse button to draw a frame around the spectral range you want to enlarge.
- If you click on the left mouse button again, the crosshair cursor disappears and you can reposition the frame.
- Click on the left mouse button to have the spectral range displayed in the spectrum window.

To reduce the enlarged range use the *Zoom → Zoom Out* command.

B Use the *Scale all Spectra → Show Everything (XY)* command to return to the original view. The *Page* back command in the *Display* menu allows to have the last 10 spectral ranges displayed again.

C The *Shift Curve* command contains different options:
   - Whole Curve (vertically)
   - Top or Bottom (stretch the curve in y direction)

   To shift the curve...
   - ...select the respective option.
   - Click on the spectrum. The cursor changes into $\text{↖}_{\text{M}\theta}$.
   - Press the left mouse button and shift the curve.
   - To deactivate the shift mode right click into the spectrum window. To undo these changes, select the *Reset* option.

D The *Crosshair* command contains two options:
   - Cursor - the cursor is displayed as crosshair
   - Follow Data - follows the data points of a spectrum, use the *Follow Data* command.

   The current crosshair position (e.g. wavelength or absorption unit) is displayed in the upper right corner of the spectrum window. This allows to easily read out the x/y positions directly from the spectrum. If you right click into the spectrum window, the *Crosshair* command is deactivated.

E The color of the spectrum can be changed. Select the appropriate color from the color palette displayed.

F The spectrum is deleted from the spectrum window.

G This command allows to identify peaks even more precisely:
   - Right click anywhere on the spectrum.
   - Select *Add Annotation* from the pop-up menu.
   - At the cursor position an arrow is inserted indicating the wavenumber of this data point.
   - If you position the cursor onto the arrow head, the cursor

     changes into ✛. Press the left mouse button to move the arrow head.

   To edit the annotation text, right click on the wavenumber and select *Properties* from the menu which pops up. The *Center text lines* and *With Arrows* check boxes are activated by default.

H Data files can be copied in different spectrum windows.

I This command allows to set single peaks. If you move the cursor to

   the desired position, the cursor changes into: ↓ . Click on the left mouse button. The wavenumber of the generated peak will be displayed. **In case of equally large peaks only the peak close to the cursor will be displayed.** After a single peak pick a ▱ data

block is generated and displayed in the browser. Single peaks set can be deleted. Right click on the wavenumber displayed for the particular peak and select the *Delete Peak Mark* option. See also chapters 2.1.4 and 3.7.5.

J General settings regarding the spectrum display can be defined by the *Properties* command. The following settings are possible:

- **Display Limits**
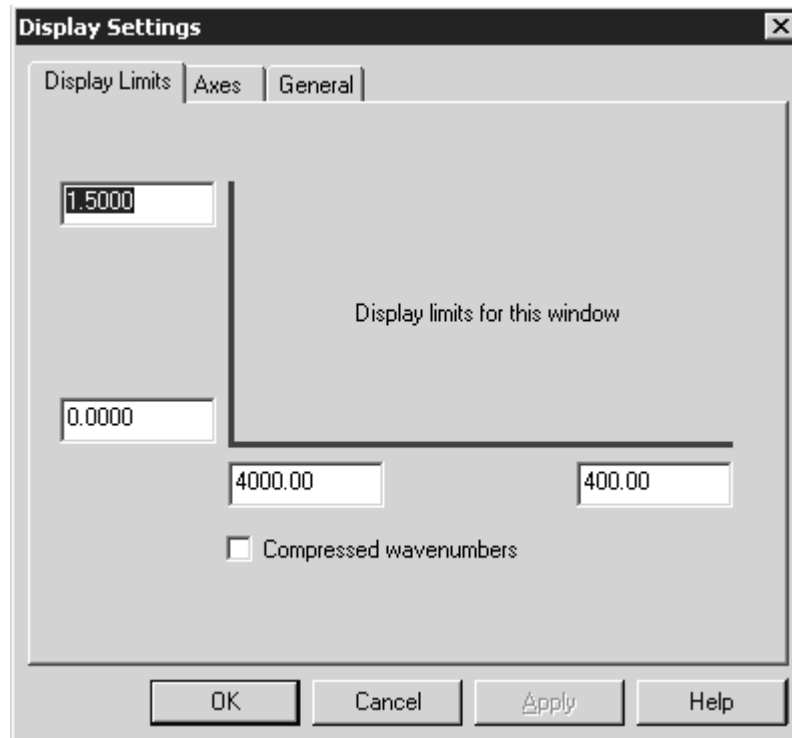
Figure 24: Display Settings - Display Limits

The *Display Limits* tab allows to change the size of the displayed region.

• **Axes**
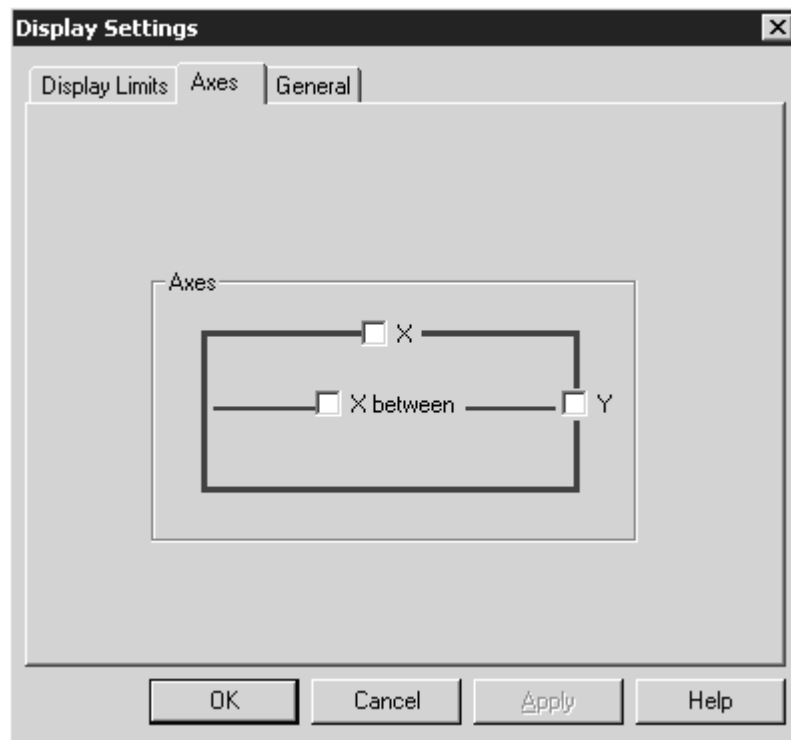
Figure 25: Display Settings - Axes

Each spectrum can be displayed with additional axes on top and on the right side of the spectrum window. If the spectrum window contains more than one spectrum and the spectra are displayed in stacked mode, you can define separate axes for each spectrum if you select the *X between* option.

• **General**
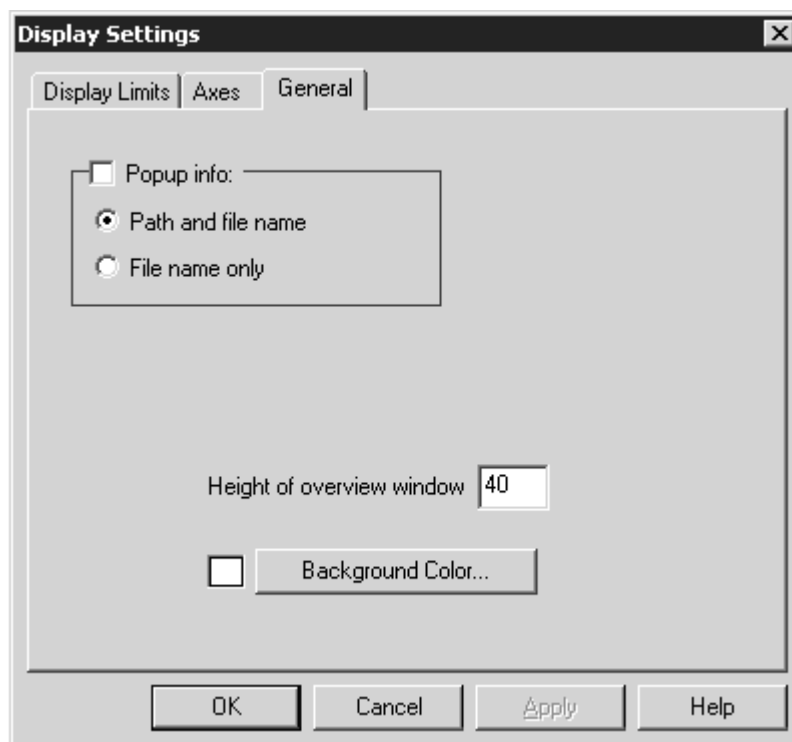
Figure 26: Display Settings - General

The *General* tab allows to change the background color and the default height of the overview window. If you activate the *Popup info* check box, the path and file name, or path name only, will be displayed as soon as you position the cursor on the spectrum.

1.14   Defining Frequency Range

In case of some OPUS manipulation or evaluation commands you have to define frequency limits first. There are several possibilities to define a frequency range:

How to define a frequency range?

OPUS commands which require a defined frequency range contain the *Frequency Range* tab. Use this tab to define the respective frequency range. Figure 27 exemplifies the possibilities provided according to the *Normalize* OPUS command.
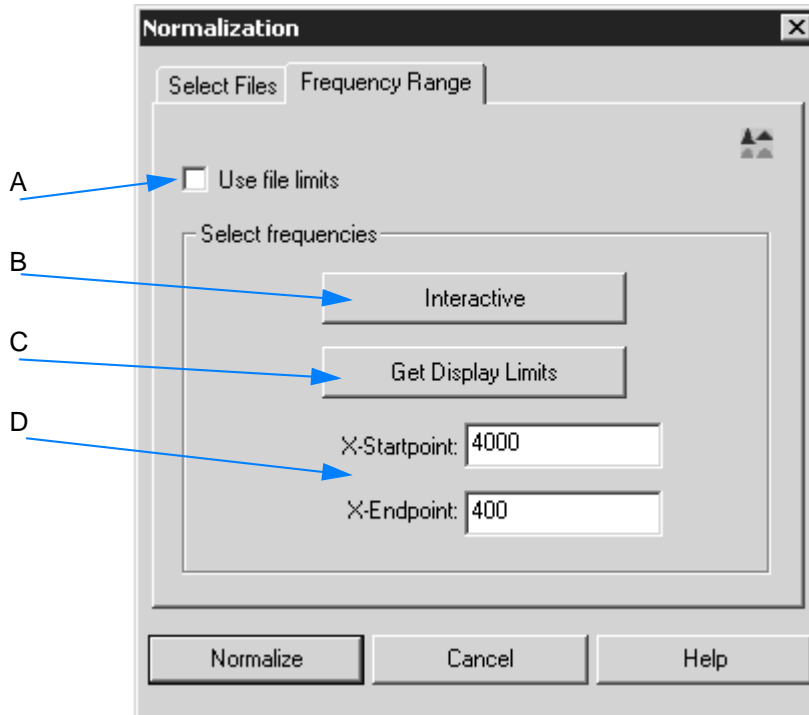
Figure 27: Select frequency range

A If the check box is activated, **the frequency range of the spectrum shown in the spectrum window** is used. The other options on the tab will be disabled.

B Use this button to i**nteractively select the frequency range**.

C The **display limits of a particular part of the spectrum** can be used as frequency range. This makes sense if you have zoomed a particular part of the spectrum before.

D **Manually enter the values for the frequency range** into the entry fields.

How to interactively define a frequency range?

1 Load the spectrum you want to manipulate or evaluate.
2 Select the respective OPUS command.
3 Click on the *Interactive* button on the *Frequency Range* tab.
4 The *Select Frequency Range(s)* dialog opens and shows the spectrum loaded.
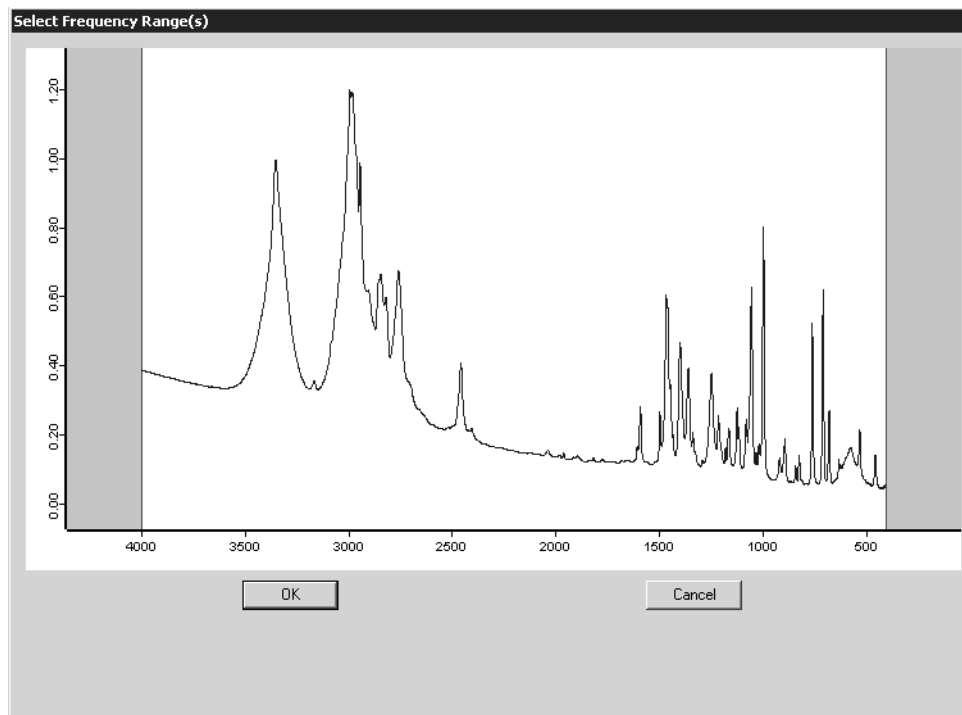
Figure 28: Interactive frequency range selection

5   Position the cursor on the boundary between the white and gray area, the cursor changes into ↔ . Press the left mouse button and move the cursor either to the left or right side.
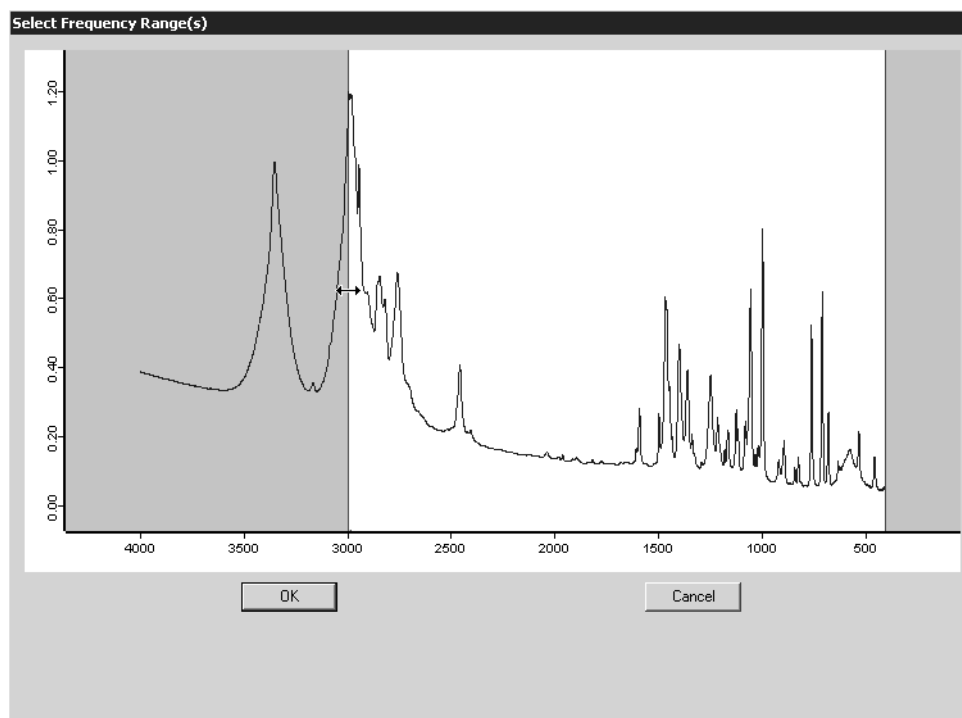
Figure 29: Select frequency range

6 Within the white section the cursor changes to ✛. Press the left mouse button to move the entire frequency range selected.
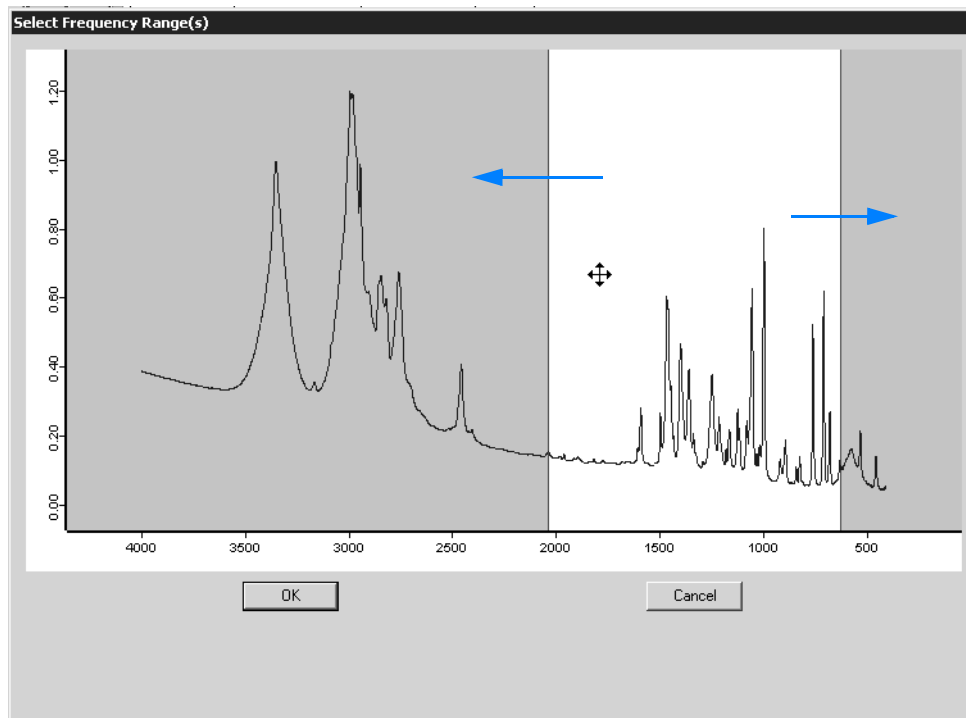
Figure 30: Move frequency range

7 Click on the *OK* button to confirm the limits of the frequency range to be used for data processing.

What does the interactive frequency range view show?

- If both frequency ranges are within the display limits, the area between the boundaries will be white, the background gray.
- If the complete frequency range displayed fits the display limits, the entire range will be white.
- If the display limits are either above or below the frequency range displayed, the background will be completely gray. In this case, close the *Select Frequency Range(s)* window, define reasonable frequency ranges and start the interactive mode again.

1.15 Information View

The information view contains measurement parameters or evaluation results of the spectrum file. This kind of data are stored in so-called report data blocks, e.g. AB or TR.

Note: If the information view is not displayed, make sure that the *Information View* option is checked in the *View* menu.

By default, the permanent information view is displayed below the spectrum window.
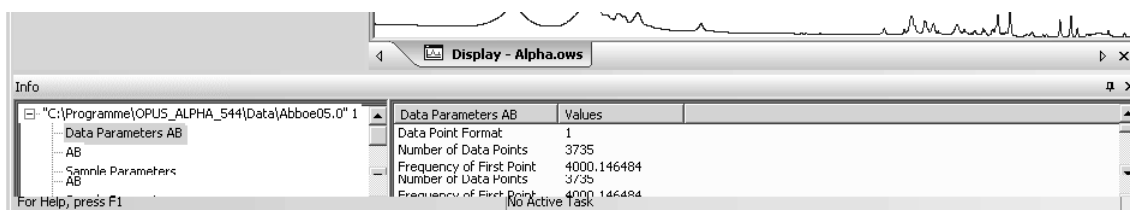
Figure 31: Information view

1.15.1 Make invisible

The ⬜ icon allows to make the information view invisible. If you click on this icon, the information view is hidden in a blue bar on the left side of the interface below the wizard.
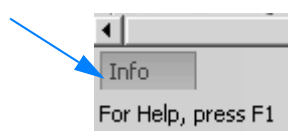
Figure 32: Invisible information view

To make the information view visible again...

...position the cursor on the blue bar. The ⬜ icon now points to the right. As soon as you move the cursor outside the information view on the OPUS interface, the view will be hidden again.

To have the information view permanently displayed again...

...click on the ⬜ icon as soon as the wizard is made visible. To close the information view click on the ✕ icon.

1.15.2 Open a separate report window

To open a separate report window double click on the respective report block in the browser. A separate report window will be displayed.
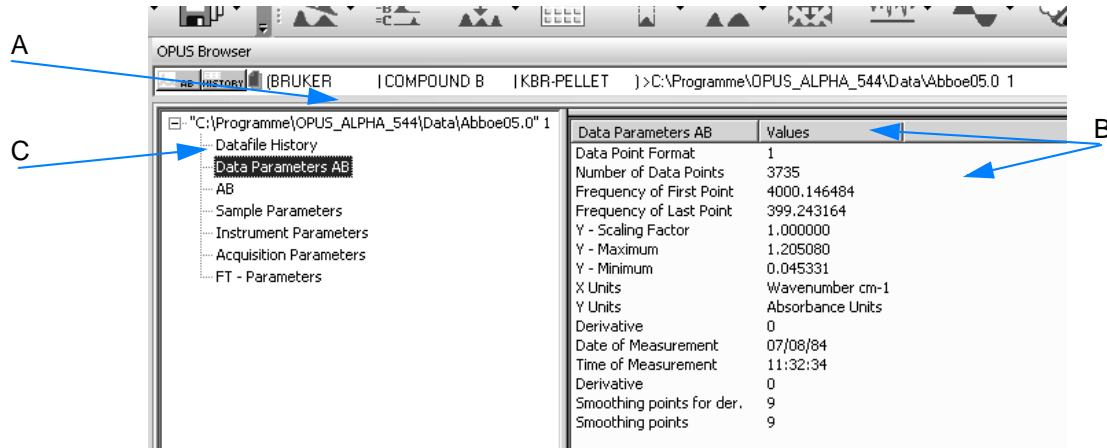
Figure 33: Report window

A Directory tree of the data included in the report block
   If you select one item in the directory tree,...

B ...the specific data are displayed on the right. Click on the column title to sort the column data in ascending or descending order.

C The *Datafile History* directory contains any manipulation made in the spectrum and changes performed in the measurement parameters. These data are recorded in a non-editable, non-deletable history datafile. Figure 34 shows such a datafile history, including several spectrum manipulations.

Figure 34: Report window - Datafile history

D The first line of the datafile history indicates the operator as well as the OPUS version and the name of the spectrum. All manipulations and their parameters are listed below in the order of their perfor-mance.

E All pieces of information are saved in the HISTORY data block together with the edited spectrum in one spectrum file. This ensures that all data manipulations can be reproduced, as every kind of manipulation as well as the operator name are automati-cally recorded.

To display the view properties set...

...right click into the report window and select the *Properties* option from the pop-up menu. The *View Properties* dialog box opens.
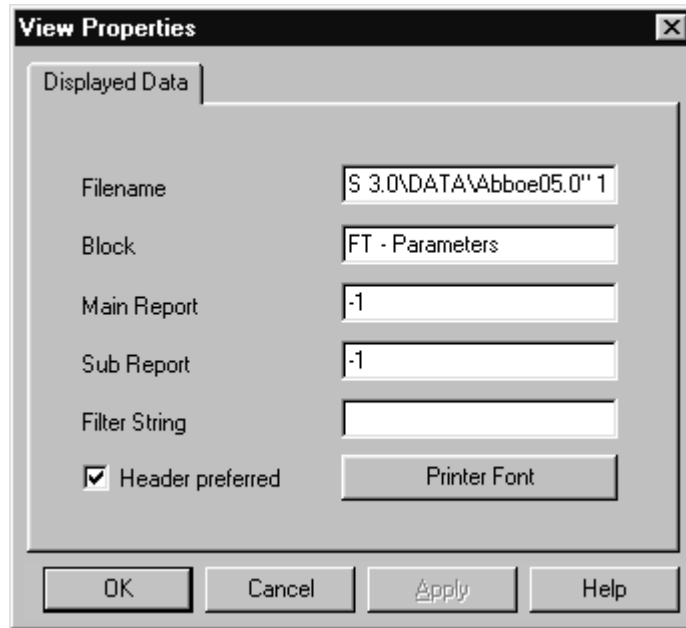
Figure 35: Information view - View Properties

The *Header preferred* check box is activated by default so that each column is provided with a header. To specify the font and font size click on the *Printer Font* button.

1.16   Instrument Status

The instrument status is shown at the right end of the status bar (   ).

- Gray: no optics connected
- Green: optics OK
- Yellow: a warning is indicated; measuring is still possible
- Red: severe error, e.g. if an optics component is defective or an instrument test has failed

If you click on the instrument status light, the *Diagnosis* dialog pops. This dialog shows the status of the single hardware components in the upper icon row. The second and third row refer to the possible active test channels. For further information on this subject refer to chapter 10.2.

1.17 File Name Extensions

The following table includes the file name extensions used in the OPUS Mentor software package.

Extension	Definition
.DAT	Pirouette file, used by InStep software
.DX	JCAMP file, also DX1, DX2
.INT	Integration method
.MTD	Library method
.NTI	Optical bench configuration file
.OWS	OPUS workspace
.PCT	Parameter correlation table used for JCAMP-DX
.PLE	Printing template
.PLT	Printing template
.Q1	QUANT method
.QCM	Quick Compare method
.RED	OPUS help file
.S01	Spectrum library, also S02, S03...

1.18 Abort OPUS

If OPUS hangs for quite some time and cannot be closed by the ✕ icon, you can abort the program by using the Windows Task Manager. **Data not stored before aborting the program will be lost.** This also applies to the workspace settings made during the program run (e.g. toolbar configuration, directory name etc.)

1   To open the Task Manager simultaneously press the *Alt*, *Ctrl* and *Del* keys on the PC keyboard. The Windows Task Manager will be displayed.

2   Select OPUS from the *Applications* tab.

3   Click on the *End Task* button. **OPUS will terminate without saving any data.**

2 Quick User Guide

The purpose of this quick user guide is to enable you to familiarize yourself with the OPUS software within a short period of time and to learn how to perform the most relevant analytical tasks on your own. This chapter describes the procedures for realizing the following analytical task definitions:

- **Sample Measurement** - How to perform a spectroscopic measurement? How to manipulate a sample spectrum? How to save and/or print a spectrum?
- **Quality Control** - Are the delivered goods or the self-made products consistent with the specified quality criteria?
- **Identification of an unknown substance** - What substance is it?
- **Quantitative Analysis** - How much of a certain component does the sample contain?

2.1 Measurement

2.1.1 General Information

It is recommended to perform a measurement using the factory parameter settings. In this case, you can start with the measurement immediately. See the following descriptions *General Measurement Procedure*.

In addition, OPUS offers you also the possibility to adapt the measurement parameter settings (e.g. the parameter value *Scan Time*) to your special demands. To do this, click in the OPUS wizard with the left mouse button next to the *Measurement* button and select the option *Setup "Measurement"...* (see figure 36). As a result, the *Setup Measurement Parameters* dialog opens. For a detailed description of this dialog window refer to chapter 3, section 3.5.
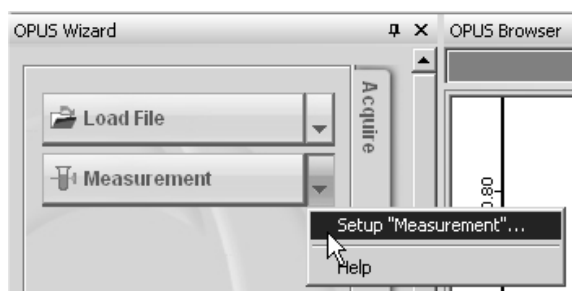
Figure 36: OPUS Wizard - Opening the Setup Measurement Parameters dialog

When measuring a sample, always pay attention to the following issues:

- If the sample needs to be prepared, due to its composition, prepare it carefully and avoid preparation errors. For information about sample preparation refer to chapter 6.
- Avoid measurement errors (e.g. the ATR crystal is not covered completely with the sample).

2.1.2   General Measurement Procedure

Generally, the measurement procedure can be subdivided into the following steps:

1   Measuring a background spectrum
2   Preparing the sample, if required
3   Measuring the sample spectrum
4   Manipulating the sample spectrum
5   Performing a peak pick, if required
6   Saving and / or printing the manipulated spectrum
7   Measuring the next sample, if required

How to perform a measurement:

1   Click in the OPUS Wizard on the *Measurement* button (see figure 37).
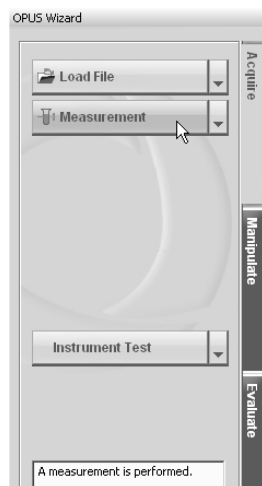
Figure 37: OPUS Wizard - Starting a measurement

2   The following dialog window opens:
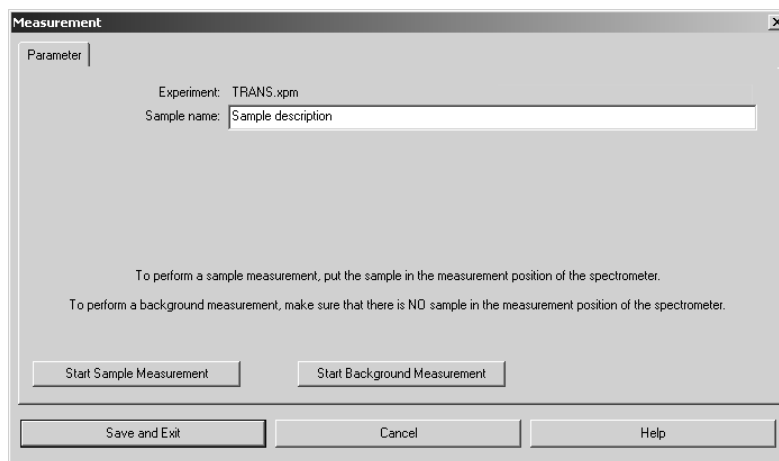
Figure 38: Measurement dialog - Starting a Background/Sample Measurement

3 First, perform a background measurement (i.e. a measurement without a sample in the spectrometer sample compartment or without a sample on the ATR crystal) by clicking on the *Start Background Measurement* button.

Note: When you acquire a background spectrum using the ATR module, first check whether the ATR crystal is really clean, i.e. it is absolutely free from residuals of the previous sample. If your sample needs to be prepared using a solvent acquire the background spectrum of the pure solvent (i.e. solvent without sample).

4 The background measurement takes a few seconds. The measurement progress is shown in the lower status bar.

5 Put the sample in the spectrometer sample compartment or on the ATR crystal.

Note: Depending on the composition of the sample (solid, powdery, paste-like, liquid etc.), the sample may need to be prepared before you can put it in measurement position of the spectrometer. For detailed information about sample preparation refer to chapter 6.

6 Then click on the *Start Sample Measurement* button (see figure 38).

7 The sample measurement takes a few seconds. The measurement progress is shown in the lower status bar. Afterwards, the acquired sample spectrum is displayed in the OPUS spectrum window.

Note: If you use the factory parameter settings, the spectrum is stored by default under *OPUS path/meas*. The file name is identical to the sample name you have entered in the *Measurement* dialog (see figure 38). If you do not enter a different sample name the file name is incremented with any further measurement.

Immediately after the sample measurement, the OPUS Wizard switches automatically to the *Manipulate* level (see the following section).

2.1.3   Manipulating a Sample Spectrum

After the sample measurement, a spectrum postprocessing may be required to ensure that OPUS yields acceptable evaluation results, for example when you intend to perform a substance identification or a quantitative analysis. For this purpose, OPUS offers a number of manipulation commands. Manipulating in this context means "optimizing" the measured sample spectrum. This section describes the following manipulation commands:

- Baseline Correction
- Atmospheric Compensation

For information about additional manipulation commands refer to chapter 3, section 3.6.

A **Baseline Correction** is always highly advisable if the spectrum baseline deviates strongly from a theoretical horizontal line. This phenomenon may occur, for example, when you measure a sample prepared as a KBr pellet. (See also chapter 6, *Sample Preparation*.) Figure 39 illustrates the effect of a baseline correction. For detailed information about this command refer to chapter 3, section 3.6.1.

Spectrum before a baseline correction

Spectrum after a baseline correction
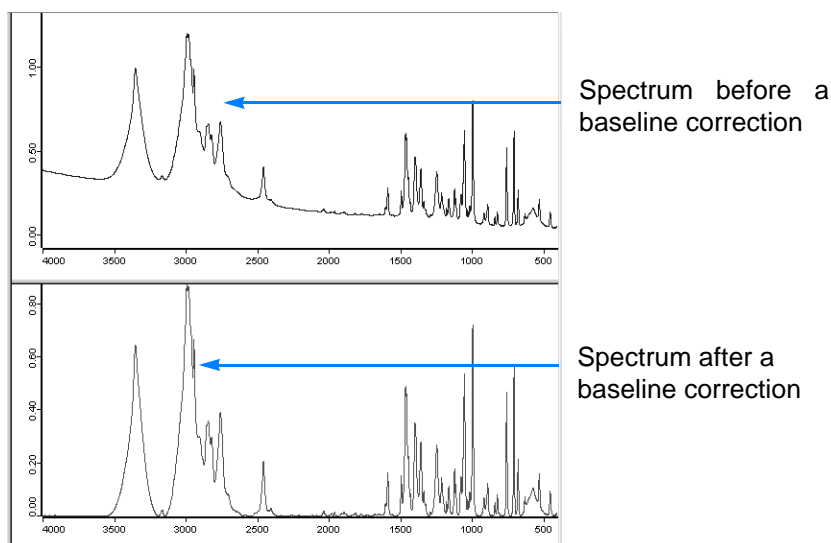
Figure 39: Baseline Correction

How to perform a baseline correction:

1   Measure a spectrum or load the file of the spectrum you intend to manipulate by clicking on the corresponding button in the OPUS wizard (see figure 37). Thereupon, the sample spectrum is displayed in the spectrum window and OPUS switches automatically to the *Manipulate* level.

2   Click in the OPUS Wizard on the *Baseline Correction* button (see figure 40).
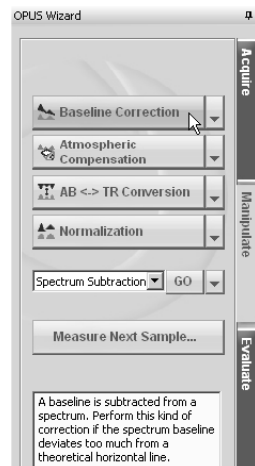
Figure 40: OPUS Wizard - Performing a Baseline Correction

  3   Thereupon, OPUS performs a baseline correction and displays automatically the corrected spectrum in the OPUS spectrum window.

Note: To undo a baseline correction, select the *Undo Changes* command in the OPUS *File* menu.

The OPUS **Atmospheric Compensation** command eliminates H_2O and/or CO_2 bands from a sample spectrum. These bands result from the ambient air and occur if there is a difference in the H_2O and/or CO_2 concentration between the moment of the background measurement and the moment of the sample measurement. Figure 41 illustrates the effect of an atmospheric compensation. For detailed information about this command refer to chapter 3, section 3.6.11.
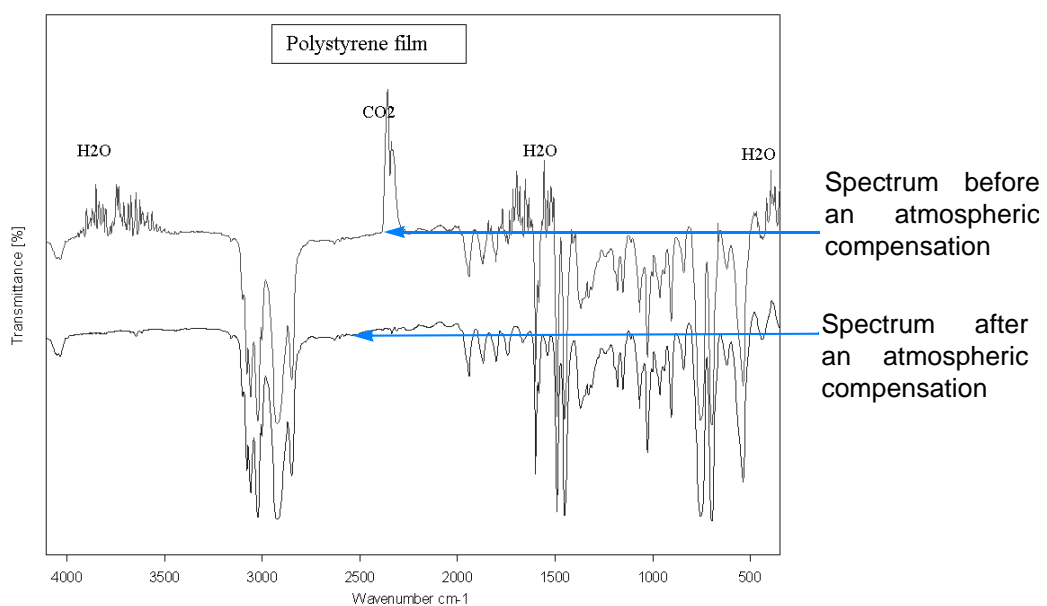
Figure 41: Atmospheric Compensation

How to perform an atmospheric compensation:

1   Measure a spectrum or load the file of the spectrum you intend to manipulate by clicking on the corresponding button in the OPUS wizard (see figure 37). Thereupon, the sample spectrum is displayed in the spectrum window (as shown in figure 42) and OPUS switches automatically to the *Manipulate* level.

Note: The *Atmospheric Compensation* command requires a spectrum file that includes, amongst others, the data blocks SSC (Sample Single Channel) and RSC (Reference Single Channel). (See figure 42.) Otherwise, an atmospheric compensation cannot be performed.

OPUS Browser with a loaded spectrum file.
This file contains, amongst others, a SSC data block and a RSC data block.
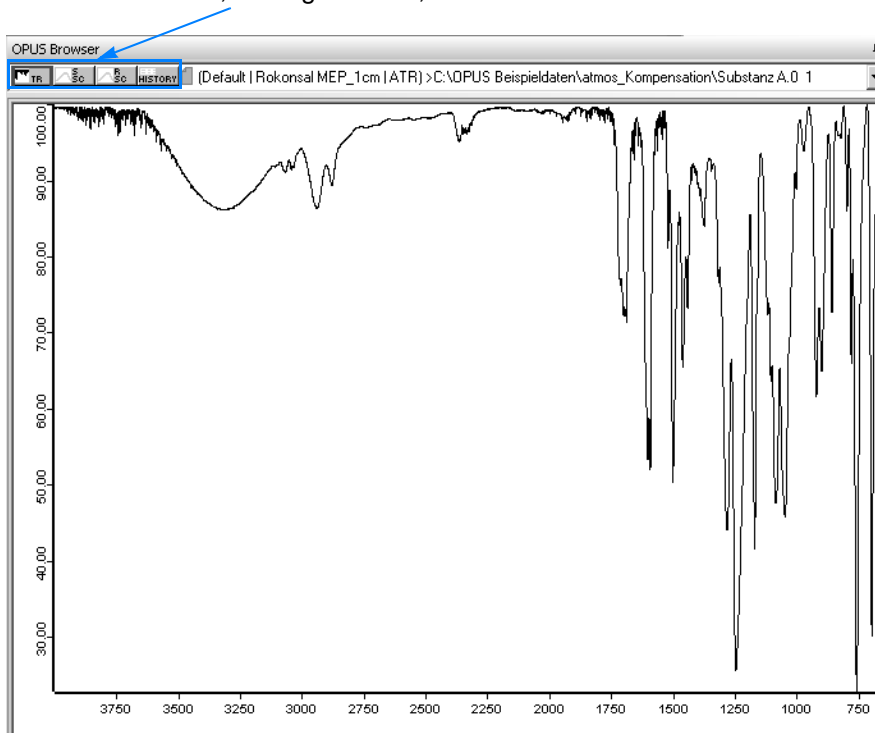
Figure 42:   Spectrum before an atmospheric compensation

2   Click on the *Atmospheric Compensation* button in the OPUS Wizard.

3   Thereupon, OPUS performs an atmospheric compensation and displays automatically the atmospherically compensated spectrum in the OPUS spectrum window (see figure 43).

Note: To undo an atmospheric compensation, select the *Undo Changes* command in the OPUS *File* menu.
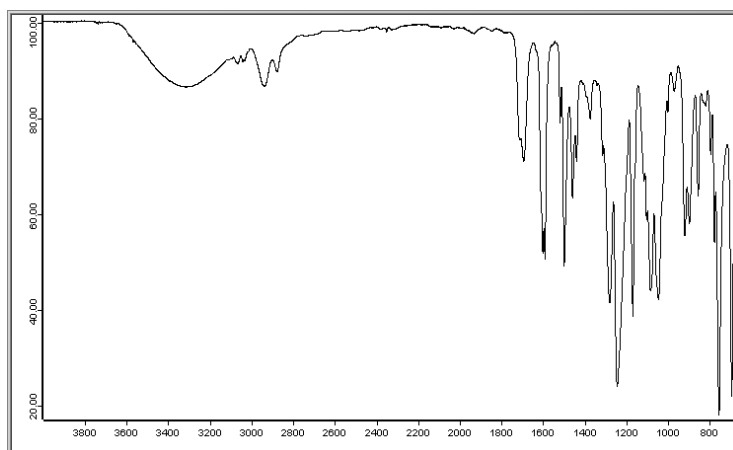
Figure 43: Spectrum after an atmospheric compensation

2.1.4   Peak Picking

The **Peak Picking** allows you a prompt determination of the exact spectrum peak positions, i.e. the exact frequency values (x-values) at which maxima (in case of an absorption spectrum) or minima (in case of an transmission spectrum) occur in the spectrum.

How to perform a peak pick:

1   Measure a spectrum or load the file of the spectrum you intend to manipulate by clicking on the corresponding button in the OPUS wizard (see figure 37). Thereupon, the sample spectrum is displayed in the spectrum window and OPUS switches automatically to the *Manipulate* level. Depending on the measurement method, the displayed spectrum is either an absorption spectrum or a transmission spectrum or an ATR spectrum.

2   Manipulate the spectrum, if required. Otherwise, click on the *Evaluate* tab and then on the *Peak Picking* button in the OPUS wizard.

3   Thereupon, the exact frequency values, at which maxima or minima occur, are displayed in the spectrum window. See figure 44a and 44b.
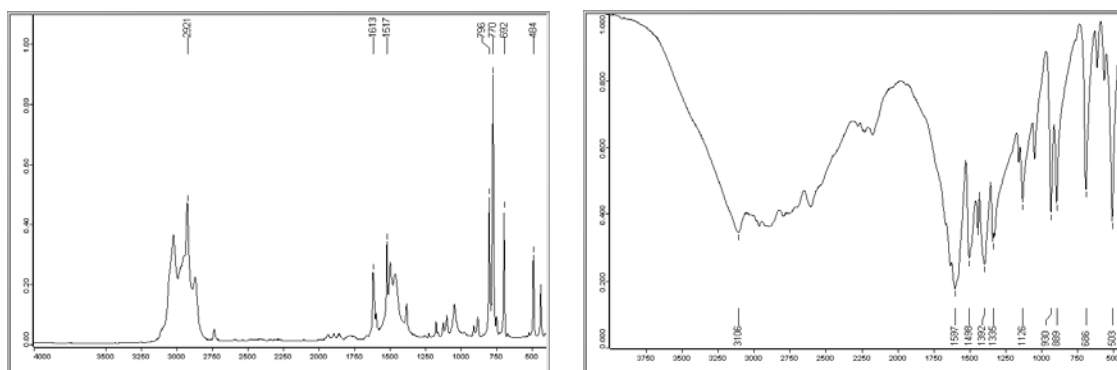
Figure 44: a)Peak pick result in case of absorption b) Peak pick result in case of transmission

How to perform an interactive peak pick:

1   Alternatively, you can pick peak(s) also interactively by clicking with the left mouse button next to the *Peak Picking* button and selecting the option *Interactive Peak Picking*. Thereupon, the following view appears:
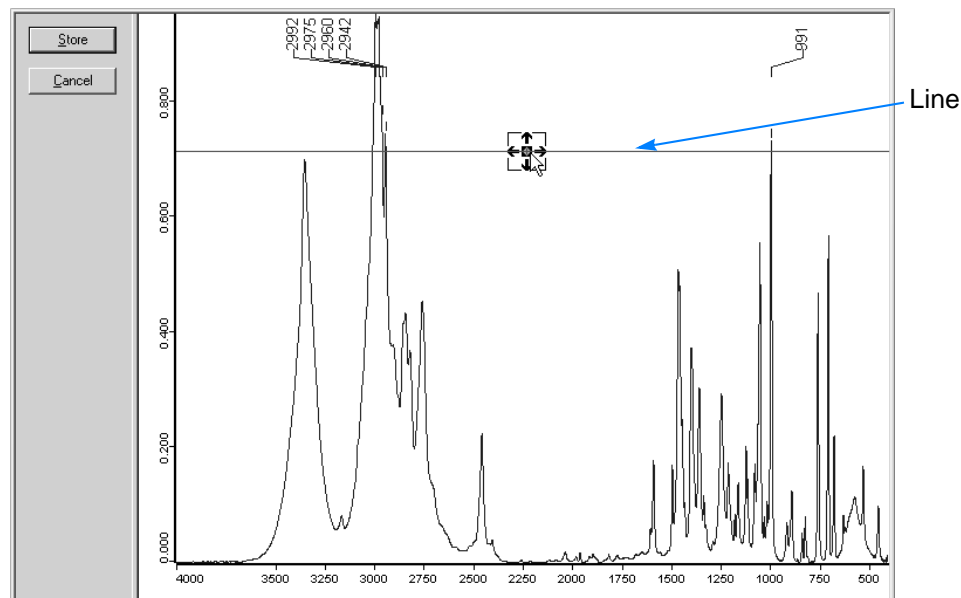
Figure 45: Interactive peak picking

2   Using the line in the spectrum window, you can select interactively the peaks of which the frequency value is of interest to you.

To do this, place the cursor on the ⊕ symbol and move the line with pressed left mouse button up- or downwards. The frequency values of all peaks above this line are displayed (see figure 45).

3   Click on the *Save* button to save the currently displayed peak position values. Thereupon, a PEAK data block is added to the spectrum file in the OPUS browser.

4   Alternatively, you can view the peak picking result in form of a report. The report is displayed below the spectrum window. See figure 46. For information about the permanent display of the information view, refer to chapter 1, section 1.15.

Peak picking result displayed in the spectrum window

Peak picking report
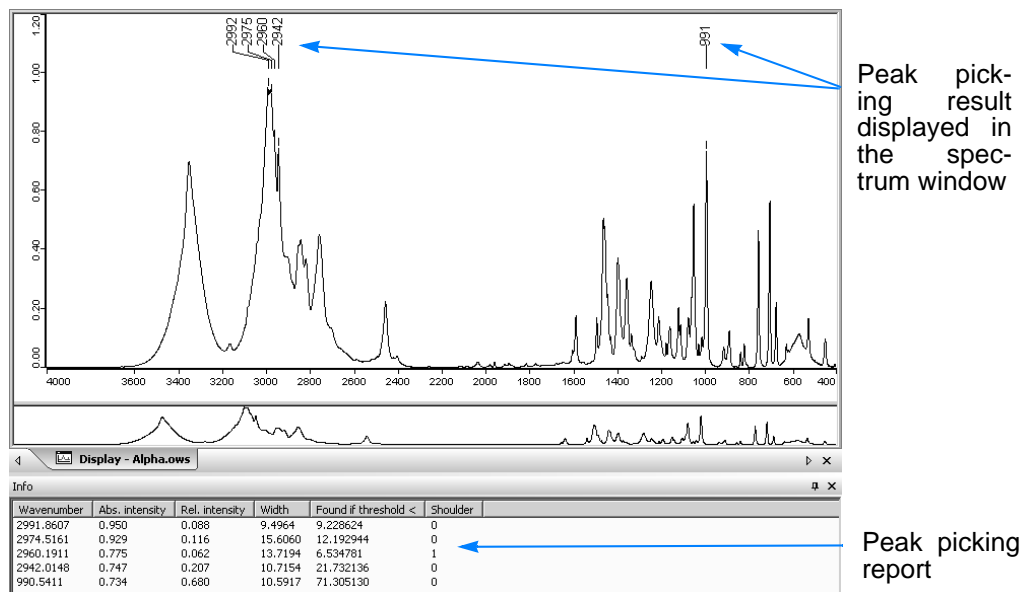
Figure 46: Peak picking report

How to perform a single peak pick:

Besides the *Peak Picking* command in the OPUS wizard, OPUS offers you also the possibility to pick specifically a single peak (i.e. to have the frequency value of a certain peak displayed) which is of interest to you. To do this, proceed as follows:

1   The spectrum in question is displayed in the spectrum window. Click with the right mouse button on the spectrum window and select in the context menu the *Single Peak Pick* command (see figure 47).
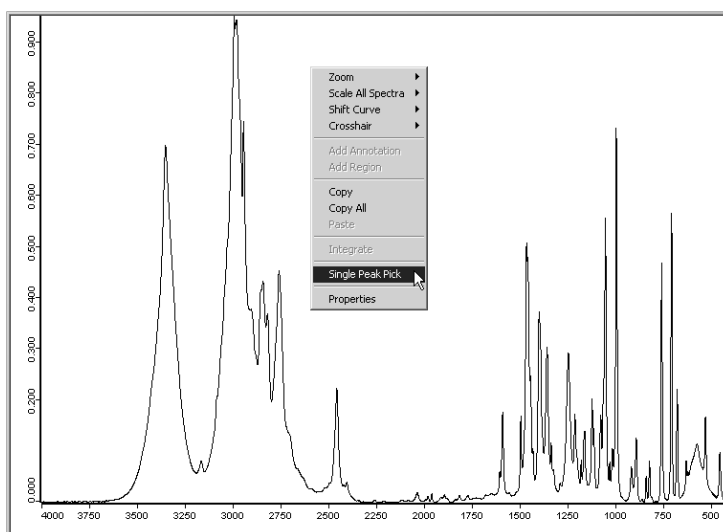
Figure 47: Single peak pick - Step 1

2   As a result, the cursor changes its appearance as follows:

3   Place the cursor on the peak which is of special interest to you and press the left mouse button. Thereupon, the frequency value of the peak in question is displayed above the peak (see figure 48). You can repeat a single peak pick as often as you like.
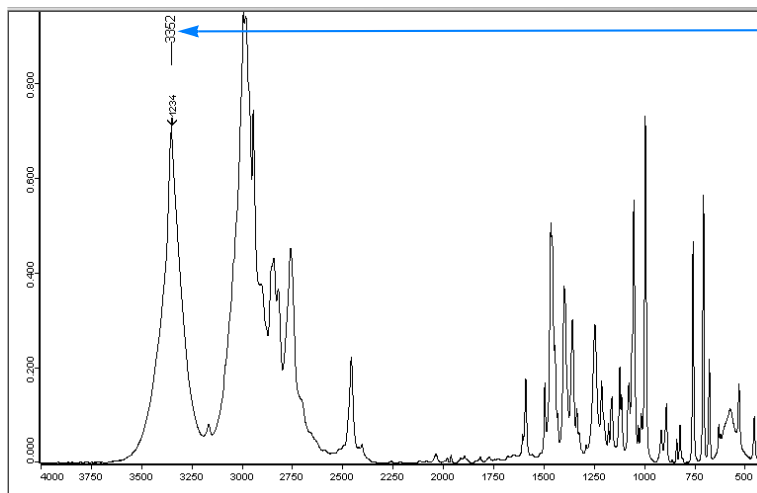
Position of an individually selected peak

Figure 48: Single peak pick - Step 2

2.1.5   Defining the next procedures

After OPUS has performed a spectrum manipulation, the wizard switches automatically to the *Evaluate* level. Depending on your particular analytical task (quality control, substance identification quantitative analysis etc.) you can now evaluate your sample spectrum using the corresponding OPUS evaluation command. The following sections 2.2, 2.3 and 2.4 provide a detailed description of the most relevant evaluation commands (Quick Compare, Spectrum Search and Quantitative Analysis). For information about all available evaluation commands refer to chapter 3, section 3.7.

After OPUS has performed an evaluation (e.g. Spectrum Search) the wizard switches automatically to the *Report* level. On this level, you decide how to deal with the current spectrum file. OPUS offers the following options:

• saving the processed spectrum and/or
• printing the processed spectrum and/or
• unloading the spectrum file and/or
• measuring the next sample.

To do this, activate the corresponding checkbox(es) and click on the *Go* button. As a result, OPUS performs automatically the selected action(s). See figure 49.
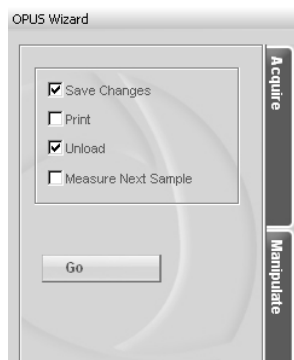
Figure 49: OPUS Wizard - Report level

How to save a processed spectrum:

1   Activate the *Save Changes* checkbox.

2   Click on the *Go* button. As a result, OPUS saves the processed spectrum with the same file name and under the same path as the original spectrum, i.e. the original spectrum is overwritten by the processed one.

Note: If you want to preserve the original spectrum select the *Save File As* command in the OPUS *File* menu and define a different file name and/or path for saving the processed spectrum.

How to print a spectrum:

1   Activate the *Print* checkbox.

2   Click on the *Go* button. As a result, the spectrum currently displayed in the spectrum window is printed.

How to unload a spectrum file:

1   Activate the *Unload* checkbox.

Note: If you want to unload a processed spectrum, it is advisable also to save it. To do this, also activate the *Save Changes* checkbox. (See section *How to save a processed spectrum.*)

2   Click on the *Go* button. As a result, the current spectrum file is unloaded from the OPUS browser.

How to start the next sample measurement:

1   Activate the *Measure Next Sample* checkbox.

Note: If you want to measure the next sample after having processed a spectrum it is advisable to save this spectrum. To do this, also activate the *Save Changes* checkbox. (See section *How to save a processed spectrum.*)

2   Click on the *Go* button. As a result, the *Measurement* dialog window (figure 37) opens again allowing you to start the next sample measurement by clicking on the corresponding button (see section 2.1.2.)

2.2 Quality Control

2.2.1 General Information

The *Quick Compare* evaluation command allows to check whether the delivered goods or the self-made products are consistent with the specified quality criteria. For realizing this task, there are the following two OPUS commands:

- **Quick Compare Setup** - This command allows to setup a quick compare method. The method setup has to be done prior to the actual *Quick Compare*.

- **Quick Compare** - This command allows to perform a *Quick Compare* using the method you have set up in advance. (*Quick Compare* implies the comparison of a sample spectrum with one or several reference spectra.)

2.2.2 The general course of quality control

Generally, quality control can be subdivided into the following steps:

1. Measuring reference sample(s) and storing the spectrum (spectra)
2. Setting up a quick compare method and saving method file
3. Measuring the sample to be analyzed
4. Performing a quick compare
5. Interpreting the quick compare result

How to choose and measure a reference sample:

For setting up a quick compare method, you first need to measure at least one or more reference spectra. In this case, reference spectra are spectra of samples of which you know for certain that they are absolutely consistent with the specified quality criteria. These samples are also called reference standards.

When choosing and measuring reference sample(s), pay attention to the following aspects:

- Use only pure samples as reference standard (i.e. samples that are free of unwanted contaminants).

- Prepare the reference standards carefully (see chapter 6, *Sample Preparation*).

- Avoid measurement errors (e.g. the ATR crystal is not completely covered with the sample).

For detailed information about how to perform a measurement refer to section 2.1.

How to setup a new Quick Compare method:

1   Click on the *Evaluate* tab and then on the *Quick Compare* button in the OPUS wizard. Thereupon, the following OPUS message appears:
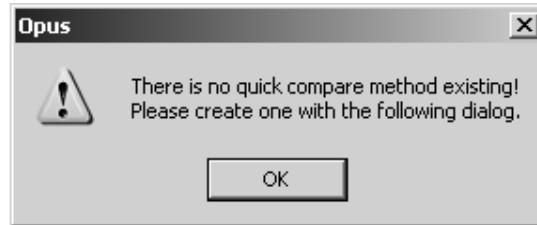
Figure 50: OPUS Message

Note: This message appears only when you click on the *Quick Compare* button for the very first time because at this stage a quick compare method has not yet be set up. Otherwise, the quick compare method set up or loaded at last is used automatically.

2   Click on the *OK* button. Thereupon, the *Quick Compare Setup* dialog window opens. See figure 51.
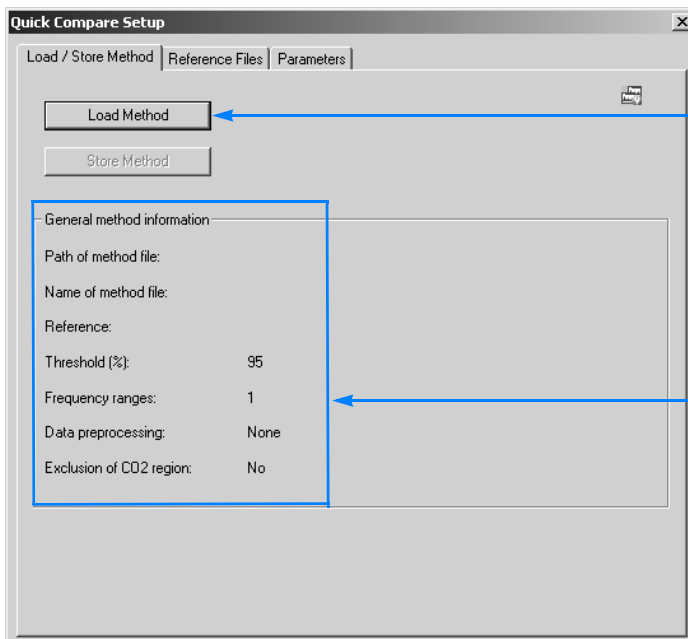
Click on this button if you want to modify an existing method file (*.QCM).

If you want to set up a new method, click on the other two tabs (fig. 52 and 53) and enter the desired parameter values. Then, return to this page of the dialog window and click on the *Store Method* button.

Note: In the upper part of this page, an overview of the parameter values you have specified on the other pages of this dialog window is shown.

Figure 51: Quick Compare Setup - Load/Store Method

3   Click on the *Reference Files* tab and select reference spectrum file(s) in question (see figure 52).
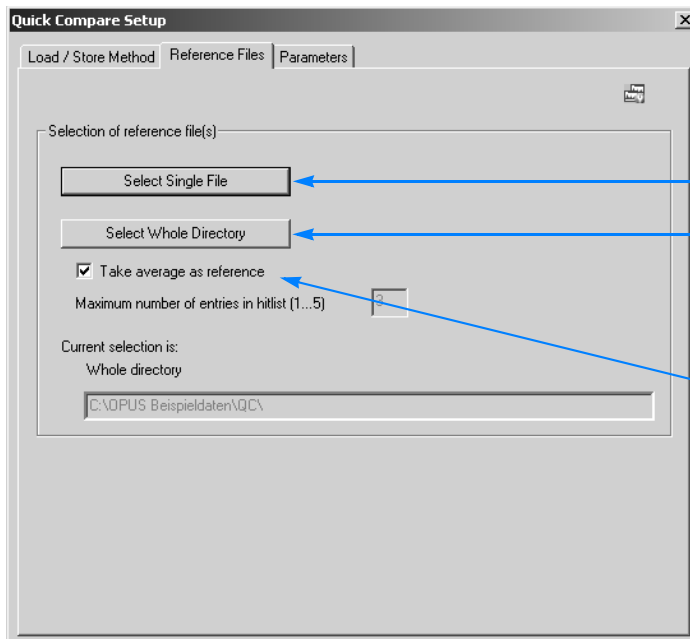
On this page, you select the reference spectrum/reference spectra for Quick Compare.

You can select either:

- only one reference spectrum or

- all reference spectra that are stored in a certain directory (In this case, the reference spectra can originate from the different sample materials.) or

- the average spectrum of all reference spectra stored in a certain directory. (In this case, the reference spectra must originate from the same sample material!)

Figure 52: Quick Compare Setup - Reference Files

> 4   Click on the *Parameters* tab and enter the desired parameter values (see figure 53).
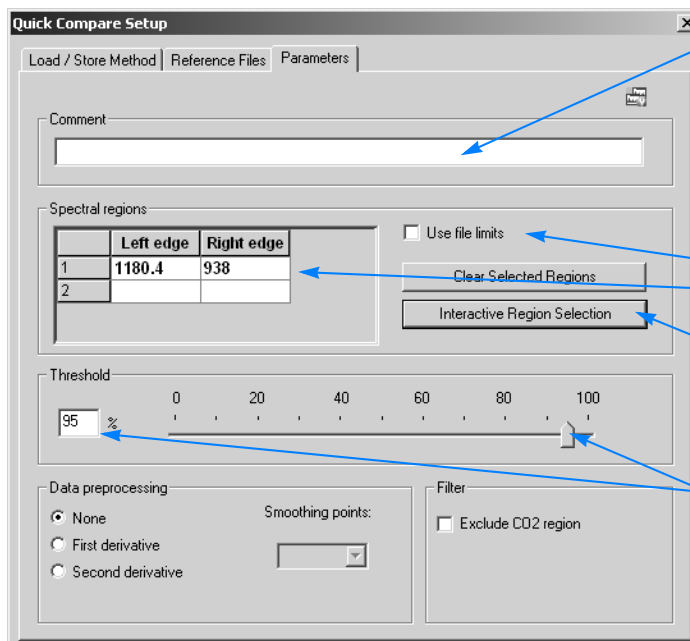
The entry of a comment is optional.

When defining the frequency region for the quick compare, you can either:

- use the file limits or,
- enter the values for one or more regions manually or
- select one or more frequency regions interactively. (See fig. 54.)

The threshold value has an influence on the quick compare result.[a] You can either set this value (in %) using the slider or enter it manually.

Figure 53: Quick Compare Setup - Parameters

a) With the threshold value, you determine the degree of similarity between the reference spectrum and the sample spectrum. In other words, you determine how similar reference spectrum and sample spectrum need to be in order that the quick compare result is OK. As a general guideline: The higher the threshold value is the higher the similarity between the reference and the sample spectrum needs to be in order to get an OK result.

> If required, you can also define a data preprocessing method (first or second derivative) and you can exclude those spectral regions from the Quick Compare in which CO_2 bands occur (between 2400 ... 2275 and 680 ... 660cm^{-1}) by activating the corresponding checkbox.

We recommend the interactive selection of the frequency region. Select those regions in which are the most relevant spectral information of the substance to be analyzed. To define further regions, click with the right mouse button on the *Select Frequency Region(s)* dialog and select the option *Add Regions* in the popup menu (see figure 54). Then, put the cursor on a boundary line of the newly added frequency region and move it with pressed left mouse button to the desired position. After having defined all relevant frequency regions, click on the OK button.
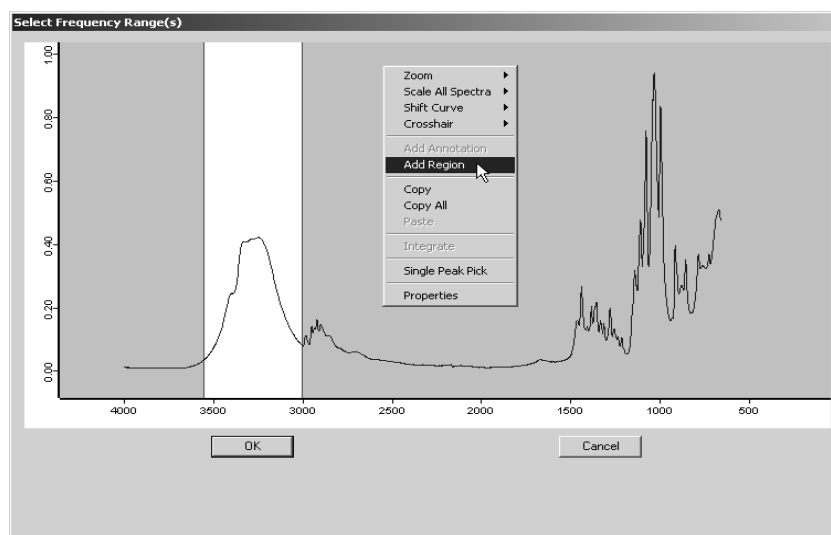
Figure 54: Interactive selection of the frequency region

5   To store the newly set-up method, click again on the *Load/Store Method* tab an then on the *Store Method* button. See figure 51.

For detailed information about this dialog window refer to chapter 3, section 3.7.

How to perform Quick Compare:

1   Measure the sample of which you want to test the quality and manipulate the sample spectrum, if required. See section 2.1. (Do not unload the spectrum yet!)

2   Click on the *Evaluate* level in the OPUS wizard.

3   Click on the *Quick Compare button*. As a result, OPUS performs automatically a Quick Compare using the method you have set up before or the method which has been loaded last.

4   Immediately after OPUS has executed a Quick Compare evaluation, the result is displayed automatically. (See figure 56, for example.)

Note: Alternatively, you can start a quick compare evaluation using the *Quick Compare* dialog window. To do this, click on the *Evaluate* level in the OPUS wizard. Then, click with the left mouse button next to the *Quick Compare* button and select the option *Select "Quick Compare" method....* Thereupon, the *Quick Compare* dialog window opens (see figure 55).

Spectrum file of the sample to be analyzed (path and file name)

Path and file name of the currently loaded method **Note: Normally, it is the method you have set up or used at last.**

Click on this button if you want to use a different method.

You can decide whether the result is to be displayed immediately after the execution of the Quick Compare and/or printed automatically by activating the corresponding checkbox(es).

Figure 55: Starting a Quick Compare

How to interpret a Quick Compare result:

The Quick Compare result is OK if the correlation value is higher than the threshold value you have determined. Analogous to this, the Quick Compare result is not OK if the correlation value is lower than the threshold value. In case of a Quick Compare evaluation, the correlation coefficient[1] r is a measure for the similarity between the two items "reference spectrum" and "sample spectrum".

Depending on what you have selected as reference for the Quick Compare (a single reference spectrum, an average spectrum or all spectra of a certain directory), keep in mind the following when interpreting the result:

- If you have selected a single file or an average as reference, you will get either an *OK* or *Not OK* as result (see figure 56, 57 and 58). In both cases, the displayed result allows you to see at first sight whether the analyzed sample meets the specified quality criteria or not (see figure 56 and 57).
- If you have selected all spectrum files of a certain directory as reference, you will not get a simply *OK* or *Not OK* as result. In this case, only those reference spectra which have a sufficient similarity with the sample spectrum, due to the threshold value you have entered and the correlation value OPUS has calculated, are displayed black. All other reference spectra which do not show a sufficient similarity with your sample spectrum are displayed gray (see figure 59)-

---

1. Normally, the correlation coefficient values can range from -1,0 (i.e. no similarity between the reference spectrum and sample spectrum at all) to +1,0 (i.e. absolutely identical spectra). For the quick compare result, this value is converted into percentage with the range $-1 \le r < 0$ being mapped to 0% and the range $0 < r \le 1$ being mapped linearly to 0% ... 100%.
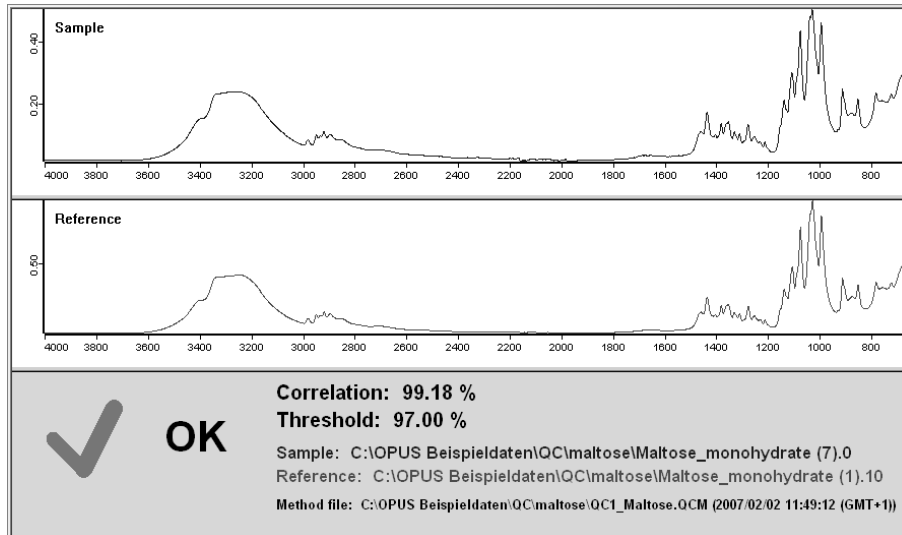
Figure 56: Result of a Quick Compare using one Reference - Sample Spectrum is OK
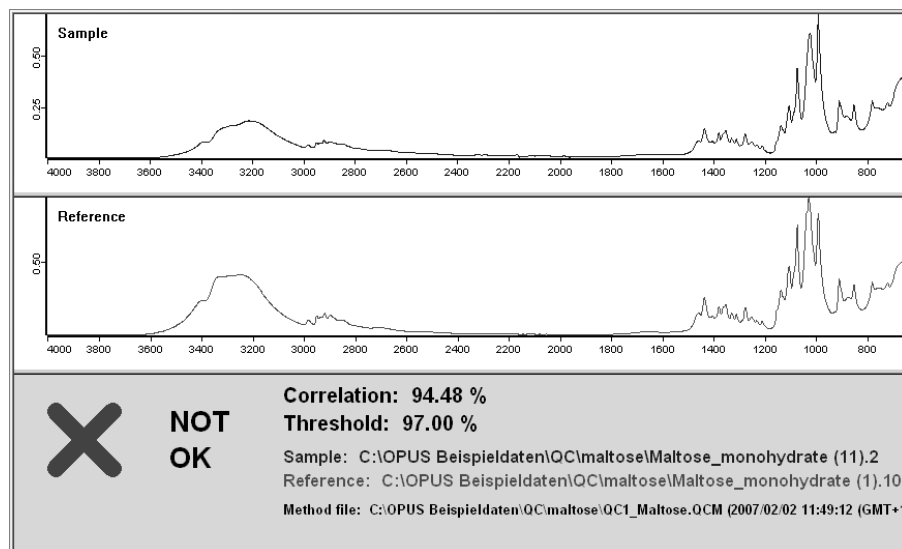
Figure 57: Result of a Quick Compare using one Reference - Sample Spectrum is not OK
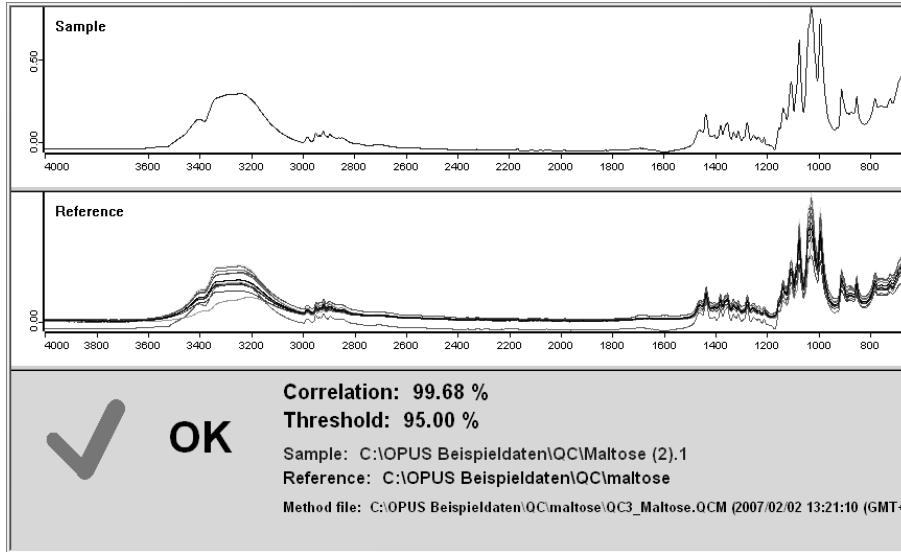
Figure 58: Result of a Quick Compare using an average as reference - Sample spectrum is OK
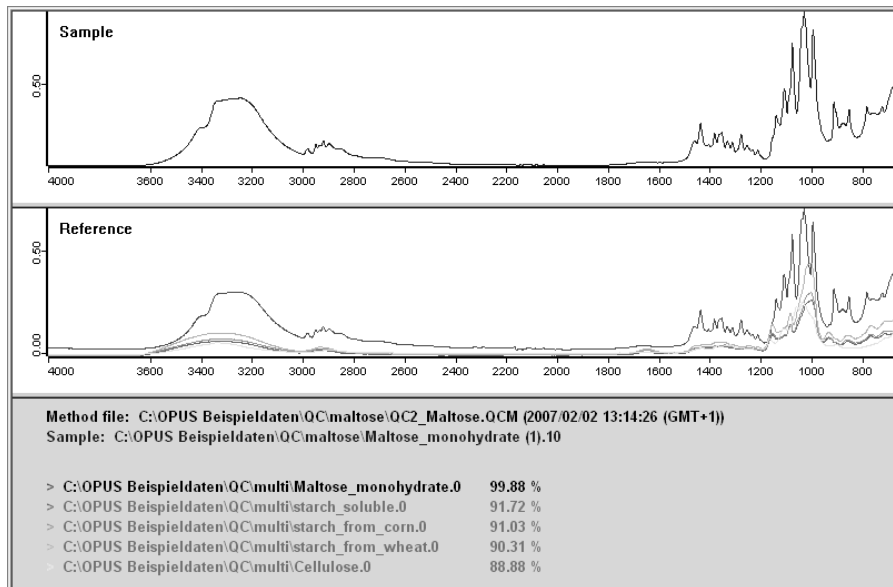
Figure 59: Result of a Quick Compare using several references - 1 hit has been found

2.3   Identification of an unknown Substance

2.3.1   General Information

The *Spectrum Search* evaluation command allows to identify an unknown substance on the basis of its IR spectrum by comparing this spectrum with the spectra of a library. Those library spectra which show an obvious similarity with the spectrum of the unknown substance are listed in a search report.

As already mentioned, a spectrum search is only possible if at least one spectra library is available. By default, the two non-commercial spectra libraries (with 350 and 200 entries, respectively) are delivered together with the OPUS programme (see figure 60). Both libraries contain spectra of a number of classes of substances (e.g. polymers, pharmaceuticals etc.).
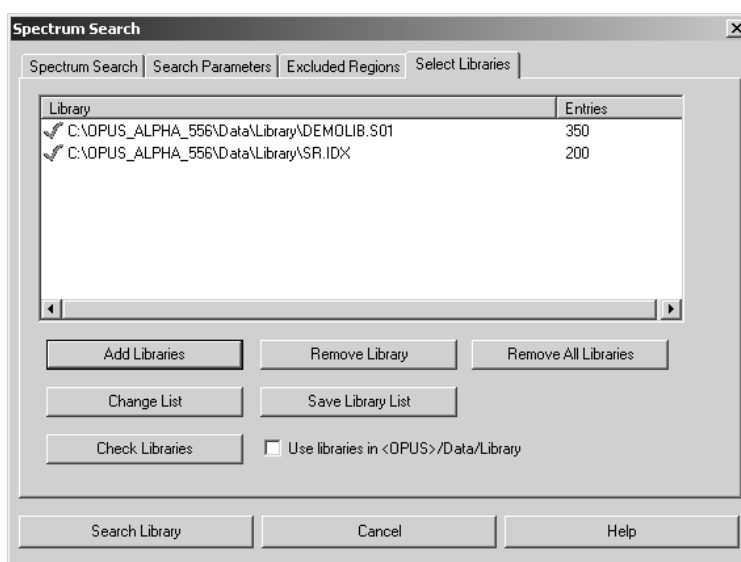
Figure 60: Available spectra libraries

> **Note: Besides the two libraries delivered with the OPUS software, Bruker also offers a number of additional spectra libraries which you can purchase.**

A decisive factor for a successful substance identification is the appropriateness of the available spectra libraries, i.e. a spectrum search can yield only acceptable results if the selected library (libraries) contain(s) entries (i.e. spectra plus additional information) of the classes of substances (e.g. polymers, pharmaceuticals etc.) that you actually analyze.

In addition, OPUS offers you also the possibility to create your own spectra library which is adapted to your special needs regarding the substances you intend to identify. See section 2.3.3 *Creating, building up and maintaining your own spectra library*.

2.3.2   The general course of a substance identification

Generally, a spectrum search in a library can be subdivided into the following steps:

1   Measuring the sample of an unknown substance and manipulating the sample spectrum, if required.

2   Starting the spectrum search.

3   Interpreting the result of a spectrum search.

How to perform a spectrum search in a library:

- Measure the sample of an unknown substance and manipulate the sample spectrum, if required (see section 2.1).

- After having executed a manipulation command, OPUS switches to the *Evaluate* level. In case you did not manipulate the spectrum, click on the *Evaluate* tab in the OPUS wizard.

- Click on the *Spectrum Search* button. Thereupon, OPUS starts the spectrum search using the factory-set search parameters. In this case, all spectra libraries that are in the directory *OPUS path/Data/Library* are searched.

  Note: OPUS offers you also the possibility to change the factory-set search parameters and/or to select different libraries. For detailed information about this topic refer to chapter 3, section 3.7.

- Immediately after OPUS has completed the spectrum search, the search report is shown (see figure 61).

How to interpret a spectrum search result:

The search report consists of 4 sub-windows (see figure 61). The lower sub-window shows the list of all hits found in the selected library (libraries). By default, the first hit in the hit list is marked and its information (spectrum, structural formula and compound information, e.g. compound name, molecular formula, molecular weight etc.) are displayed in the upper three sub-windows. To see this kind of information for another hit, click in the hit list of the hit of which you want to see more information.
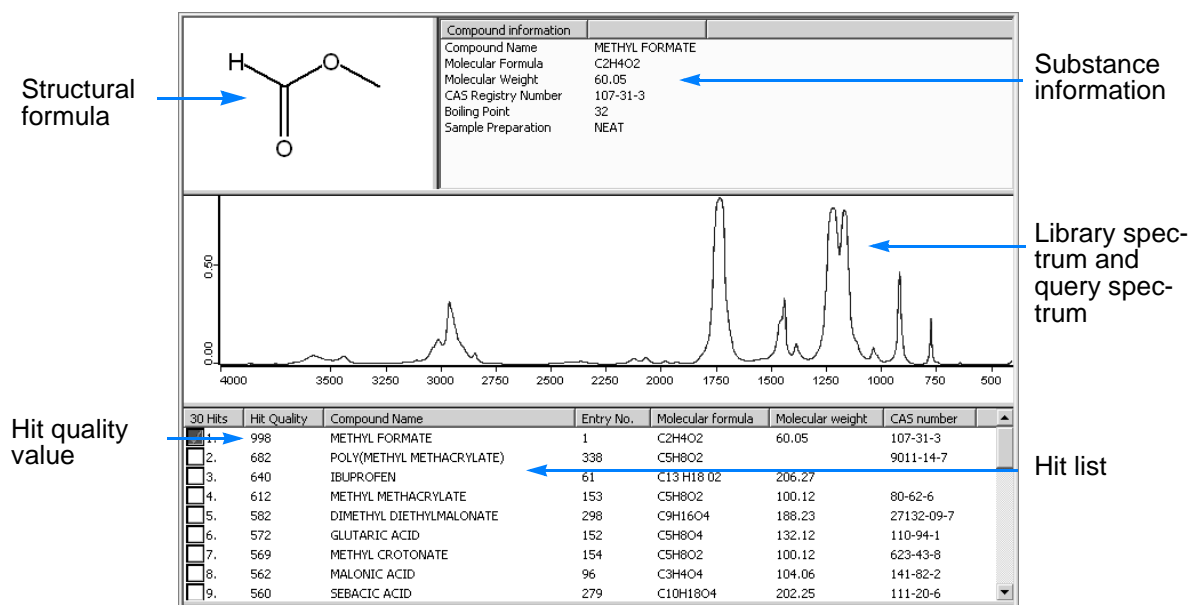
Figure 61: Spectrum Search report

- The hit quality value in the hit list gives you a general clue to what extent the spectrum of the unknown substance (also called query spectrum) resembles the library spectrum.

- The hit quality value can range from (i.e. resemblance at all) to 1000 (i.e. absolute conformity of the library spectrum with the query spectrum). The hit list is sorted according the hit quality value, i.e. the hit with the highest quality value ranks first in the hit list.

- Moreover, you can compare visually the query spectrum with the library spectrum to find out whether there is a certain resemblance between the two spectra.

2.3.3   Creating, building up and maintaining your own spectra library

Besides the usage of the delivered and/or commercial spectra libraries, OPUS offers you the possibility to create your own library that suits your specific analytical needs.

For creating, building up and maintaining your own spectra library, the following OPUS commands are available:

- Initialize Library
- Store Spectrum in Library
- Library Editor
- Library Browser

For detailed information about these commands refer to chapter 3, section 3.7.

When creating your own spectra library, pay attention to following aspects:

- When choosing the samples for the library, try to cover the hole range of the class(es) of substances you want to analyze with this library in the future. Keep in mind the following: The more extensive and diverse the library is, the better the search result will be.

- Use only pure substances (i.e. substance that are free of unwanted contaminants).

- Prepare these samples carefully (see chapter 6, *Sample Preparation.*)

- Avoid measurement errors (e.g. the ATR crystal is not covered completely with the sample).

- Before adding the measured sample spectra to the library, optimize them adequately using the available manipulation commands.

- Add preferably absorption spectra[1] to the library.

- Think already in advance of the additional information you want to include in the library and make sure that they are available.

The above mentioned aspects are crucial preconditions for the creation of a library that is to yield acceptable search results for future analyses.

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1. In an IR spectrum, the position and intensity of the absorption bands are very substance-specific. Similar to a human fingerprint, the absorption spectrum of a substance is well-suited for the identification of it.

2.4   Quantitation of a Sample Component

2.4.1   General Information

If your sample is a mixture of several components (e.g. a tablet containing several active agents) OPUS allows you to quantitate one of these components which is of special interest to you (e.g. the quantity of active agent A contained in the tablet). For realizing this task, there are the following two OPUS commands:

- *Quant Builder* - for setting up a QUANT method and
- *Quantitative Analysis* - for performing the actual quantitative analysis

When you perform a quantitative analysis, it is highly recommended that you normalize all spectra (i.e. both the calibration spectra and the spectra of the sample(s) you intend to analyze) before the evaluation. Spectra normalization is an OPUS manipulation command. Normalizing means that the spectra are scaled to that effect that the minimum and/or maximum of the spectra assume the same value. In doing so, the spectra can better be compared with each other. Especially in case of ATR spectra, a normalization is highly recommended. For detailed information about this command refer to chapter 3, section 3.7.

2.4.2   The general course of a quantitative analysis

Generally, a quantitative analysis can be subdivided into the following steps:

1. Getting a set of about 5 samples and determining the exact concentration values of the sample component in question using a different technique (e.g. weighing). These samples are also called calibration samples. They are required for setting up the QUANT method.
2. Setting up a QUANT method using the OPUS command *Quant builder* and the calibration samples.
3. Performing a quantitative analysis using the QUANT method you have set up before and the OPUS command *Quantitative Analysis*.
4. Interpreting the analysis.

When choosing the calibration samples, pay attention to the following aspects:

- Ideally, the calibration sample set should contain at least 5 samples.
- Make sure that the concentration value of the component in question differs from calibration sample to calibration sample.

How to setup a QUANT method:

1 Measure one of the calibration samples and manipulate the sample spectrum, if required (see section 2.1). Keep the spectrum file loaded in the OPUS browser.

2 Click on the *Evaluate* tab in the OPUS wizard, select the option *Quant Builder* in the drop-down list and click on the *Go* button. Thereupon, the *Quant Builder - New* dialog window opens (see figure 62). The dialog window already includes the path and the file name of the currently loaded spectrum file.

3 Enter the name of the component to be analyzed.

4 Specify the unit of the measurement (e.g. mg, ml, %) for the concentration value. **Note: The unit of measurement you enter in this dialog depends on the unit in which you have determined the concentration values of the calibration sample before. And the result of the quantitative analysis is displayed in this unit as well.**

5 Enter the exact component concentration value for the calibration sample in question. **Note: You need to have determined this value before using a different analytical technique.**
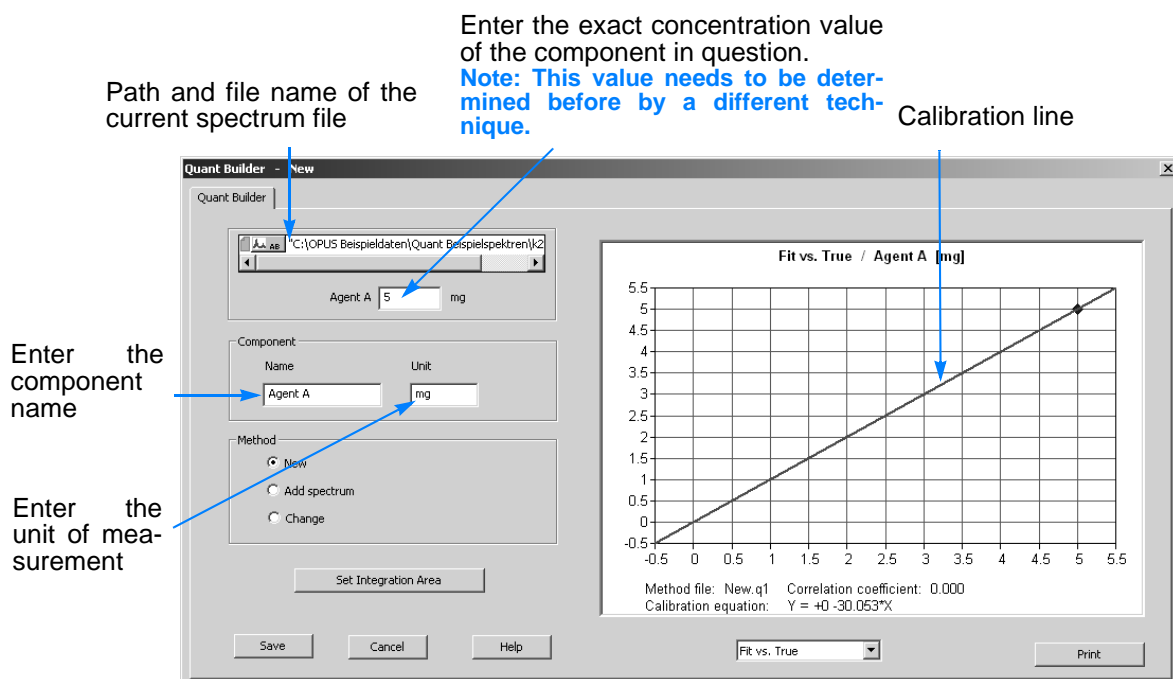
Figure 62: Dialog Window Quant Builder

Already at this stage (i.e. on the basis of one calibration spectrum and its corresponding concentration value), OPUS calculates a calibration line[1] (see figure 62). In the further course of the QUANT method setup, this calibration line will be improved by adding the data of the other calibration samples.

Note: When you add the first calibration spectrum to a new QUANT method, make sure that the *New* option button is activated.

6   Click on the *Set Integration Area* button. Thereupon, the window shown in figure 63 appears allowing you to set an integration area and select an integration method.

Note: Set the integration area in such a way that the spectral band resulting from the component in question is within integration area. For this reason, it is recommended to set the integration area not until at least 3 or 4 calibration spectra have been added to the QUANT method because only at this stage you can recognize clearly the spectral band resulting from the component in question (see figure 64).

Spectral band resulting from agent A

Note: You can change the integration area boundaries interactively by placing the cursor on a boundary and shifting it with pressed left mouse button.
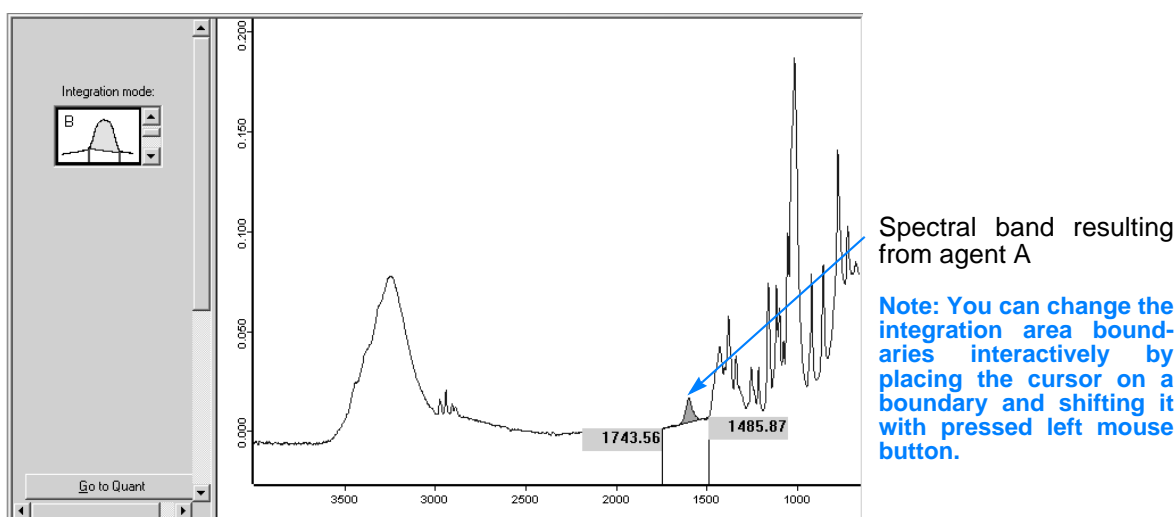
Figure 63: Defining the Integration Area and the Integration Method

7   Now click on the *Go to Quant* button in order to return to the *Quant Builder* dialog window.

8   Click on the *Save* button. As you are setting up a new QUANT method, OPUS prompts you to enter file name and path under which the method file is to be saved. Enter a file name, specify the path and click on the *Save* button.

9   Thereupon, the *Quant Builder* dialog window disappears.

10   Measure the next calibration sample by clicking on the *Measure Next Sample...* button in the OPUS wizard (see section 2.1).

---

1. The calibration line visualizes the relation between the calibration spectra and the corresponding concentration values of the component in question. For the quantitation of a certain component, OPUS calculates the quantity of this component on the basis of the spectrum of the sample to be analyzed and the calibration line.

11 Open the *Quant Builder* dialog again by clicking in the OPUS wizard on the *Evaluate* tab, selecting in the drop-down list the option *Quant Builder* and clicking on the *Go* button.

12 Enter the component concentration value of the calibration sample in question.

Note: For the second and every following calibration sample, you do not need to enter component name and unit again.

13 When adding the second or any further calibration spectrum to the existing QUANT method, make sure that the *Add spectrum* option button is activated.

14 To add the data of the second calibration sample to the QUANT method, click on the *Save* button. Thereupon, the *Quant Builder* dialog window disappears.

15 Repeat step 10 to 14 for the remaining calibration samples.

Only after you have added 3 or 4 calibration spectra to the QUANT method is it recommended to set the integration area. To do this, activate the *Change* option button and click on the *Set Integration Area* button. Thereupon, the window shown in figure 64 appears.
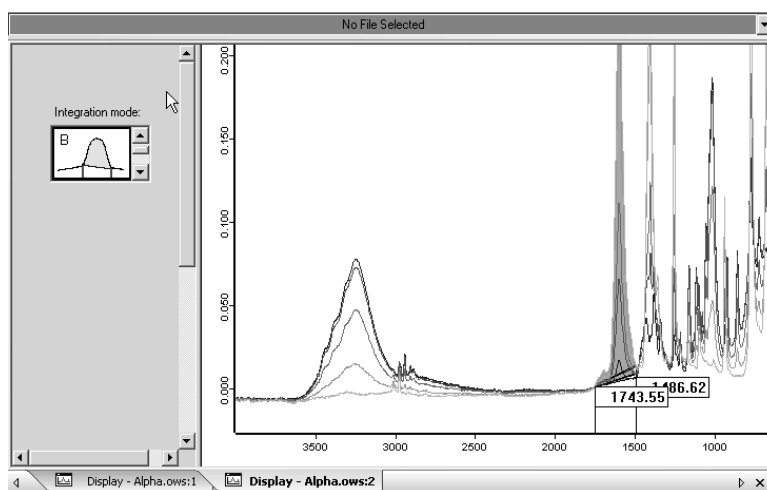
Figure 64: Defining the integration area on the basis of several calibration spectra

At this stage, the window includes all calibration spectra added to the QUANT method so far. The display of several calibration spectra enables you to set the integration area because now the band resulting from the component to be quantified is clearly recognizable due to differences in the band height because the band height is quantity-dependent.

For detailed information about the *Quant Builder* command refer to chapter 3, section 3.7.

How to perform a quantitative analysis:

1   Measure a sample of which you want to quantitate a certain component. For information about how to perform a measurement refer to section 2.1.

2   Click on the *Evaluate* tab an then on the *Quantitative Analysis* button in the OPUS wizard. Thereupon, the *Quantitative Analysis* dialog window opens. See figure 65.

Spectrum file of the sample to be analyzed (path and file name)

Path and file name of the currently loaded QUANT method **Note: Normally, it is the method you have set up or used at last.**

Click on this button if you want to use a different QUANT method.
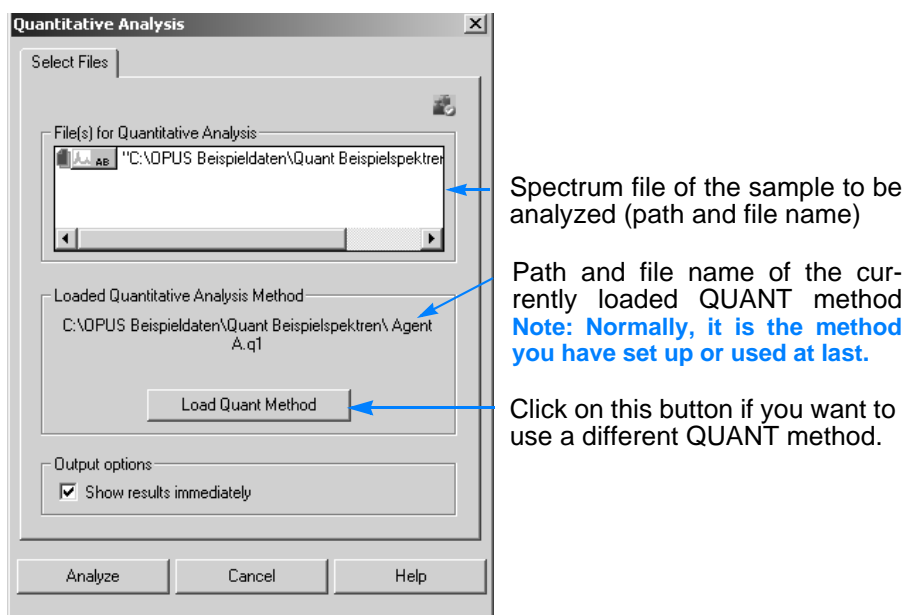
Figure 65: Quantitative Analysis dialog

3   The sample spectrum file is already included in the *File(s) for Quantitative Analysis* field.

4   The QUANT method you have set up or used at last is already loaded. In case you want to use a different method click on the *Load Quant Method* button and select the QUANT method file (*.q1) you intend to use.

Note: You can perform a quantitative analysis using either:

- **a newly set-up method or**
- **an existing method you have modified or**
- **an existing method you select explicitly or**
- **the method which has been loaded last.**

5   Make sure that the *Show results immediately* button is activated (see figure 65). In this case, the result is shown immediately after OPUS has completed the evaluation. The result is displayed in form of a report (see figure 66).

Note: In case this check box has not been activated double-click on the QUANT data block of the spectrum file in order to display the quantitative analysis result.

6   Finally, click on the *Analyze* button.

How to interpret a quantitative analysis result:

Result of QUANT evaluation:

Component	Prediction	Sigma	Unit	Integr. Result
Agent A	79.41	4.93	mg	2.89

Figure 66: QUANT Report - Result of a quantitative analysis

The QUANT report delivers the following information:

- name of the component that has been quantitated
- concentration value (prediction) of the component in question calculated by OPUS
- standard deviation (sigma[1]) of the calculated prediction value
- unit in which the calculated concentration value is given

Note: You have specified this unit when setting up the QUANT method.

- the integration result for the spectral band which results from the component to be quantitated.

---

1. Sigma is the standard deviation of the calculated concentration value. The sigma value is determined by the quality of the QUANT method you have set up. Ideally, the sigma value should be as small as possible.

3 OPUS Commands

This chapter describes all OPUS commands included in the different menus.

Note: Generally, the commands available in the menu depend on the workspace defined. Individually defined workspaces may not include all OPUS commands described in this chapter.

3.1 File Menu

The *File* menu includes features required for your data file management. Apart from basic commands such as loading, saving, printing and sending, the *File* menu allows to create a lab journal.
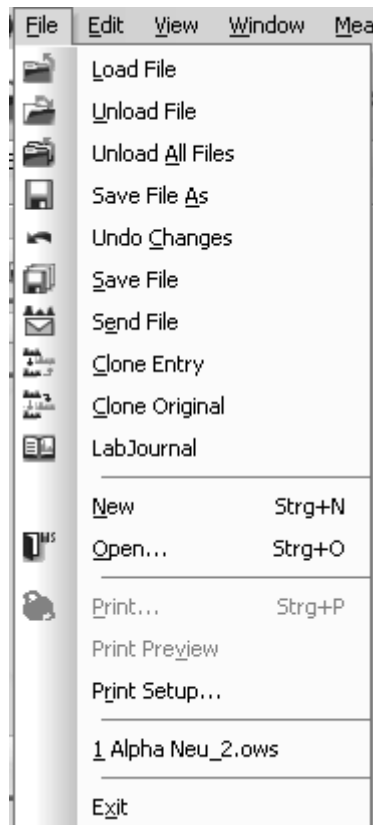
Figure 67: File Menu

3.1.1 Load File 📂

This command is used to load a spectrum file into the spectrum window. If you select this command from the menu, the following dialog opens:
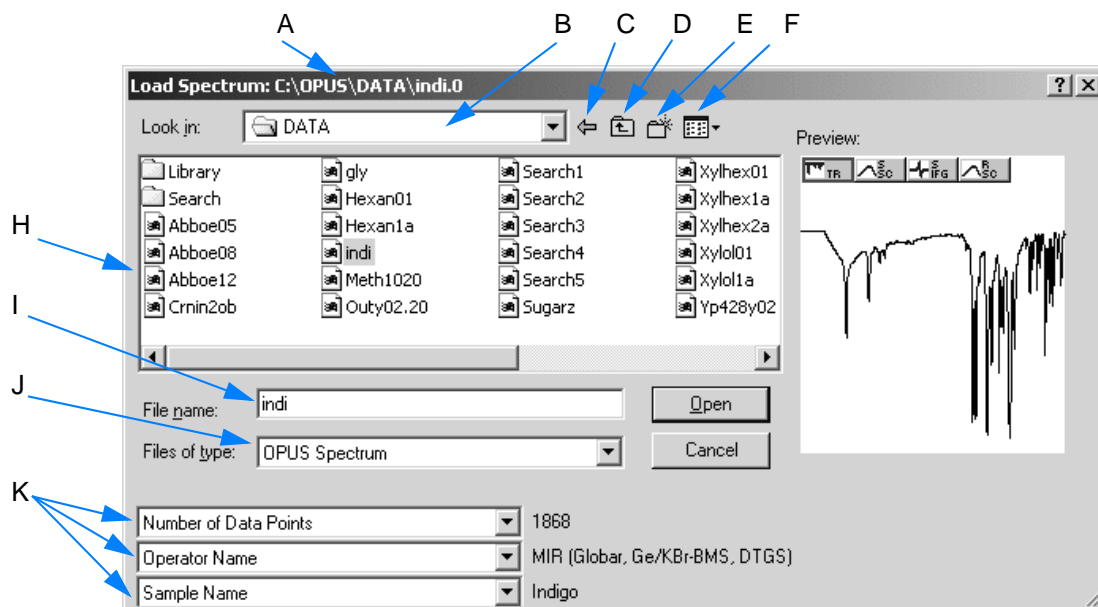
Figure 68: Load File

A **Title bar:** shows the directory in which the file is stored.

B Includes directory paths to search for spectra files.

C To return to the last selection.

D To return to the parent directory.

E To create a new directory.

F Various options to display the file list.

G **Preview window:** displays a small spectrum range without indicating the axes. Data blocks are displayed on top of the preview window. They include additional information on the spectrum file.

H File list of the path selected.

I The name of the file you want to load can be manually typed into this entry field.

J It is also possible to load spectra of different formats, e.g. JCAMP-DX or GRAMS.SPC files. These files will automatically be converted into the OPUS file format.

K Parameters are additional information appended to the OPUS file. Sometimes not all parameters to be selected by each drop-down list will be defined for each spectrum file. This means that some parameter fields may remain empty.

To open the online help click on the F1 key.

3.1.2   Unload File

Definition	The *Unload File* command removes files from the OPUS browser and spectrum window. **Note: When unloading files they will not be automatically deleted from hard disk.**
Principle	Select the file and click on the *Unload File* command.

3.1.3   Unload All Files

Definition	The *Unload All Files* command removes all files from the OPUS browser and spectrum window.
Principle	If you have loaded several spectrum files and you want to remove them all at once, select the *Unload All Files* command. A dialog opens which automatically contains the names of all spectrum files in the *File(s) to unload* selection field. Click on the *Unload* button.

3.1.4   Save File /Save File As

Definition	The two commands are used to save spectrum files.
Principle	The *Save File* command automatically saves the spectrum file and changes made into the appropriate directory. If you use the *Save File As* command you can change the directory path of the spectrum file to be saved, or export OPUS data.

If you select the *Save File* command, the following dialog opens:
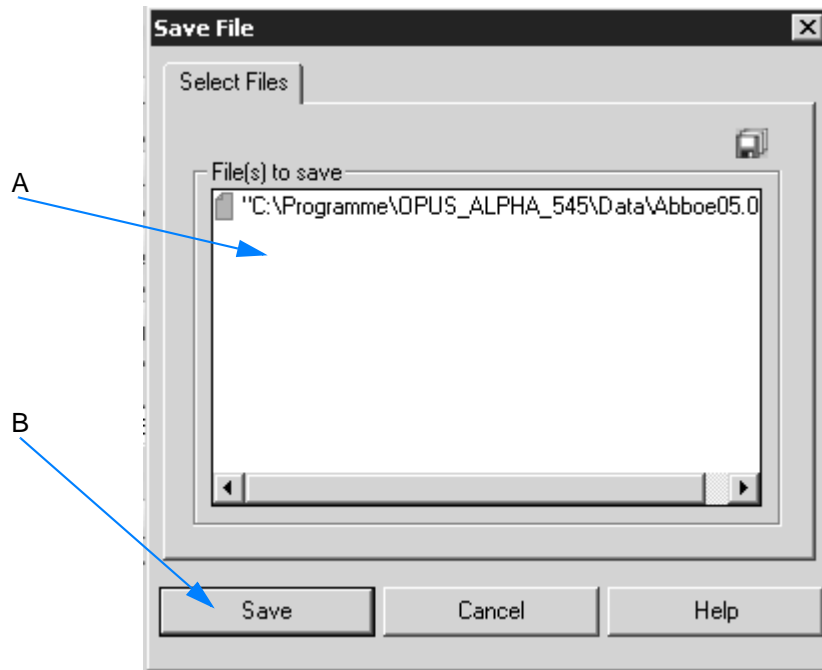
Figure 69: Save File

A The name of the spectrum file lately used is automatically shown in the *File(s) to save* selection field.

B Click on the *Save* button to save the spectrum file.

If you select the *Save File As* command, the following dialog opens:
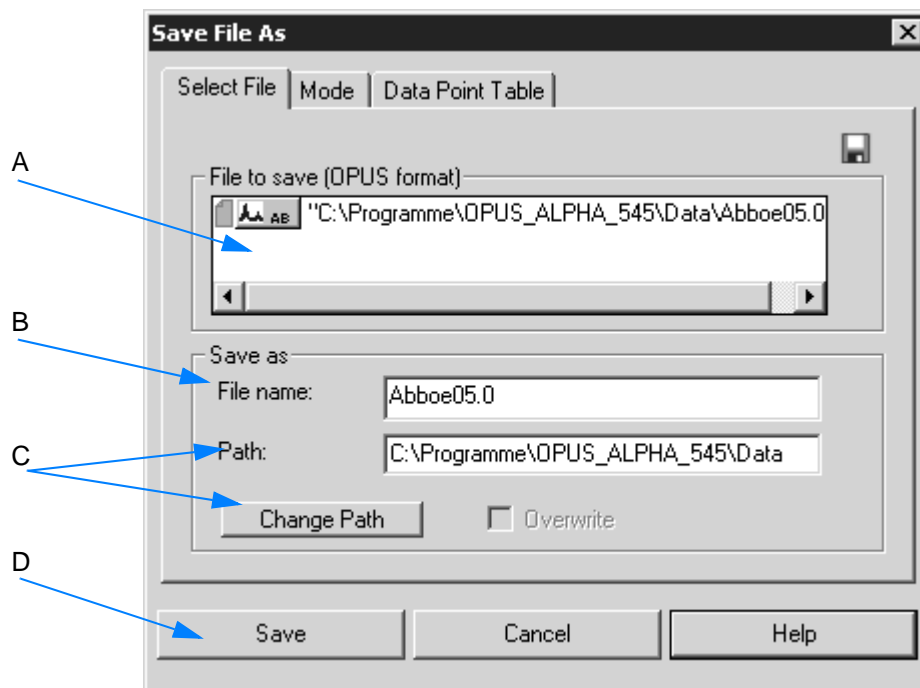
Figure 70: Save File As

A The name of the spectrum file lately used is automatically shown in the *File to save* selection field.

B Enter the appropriate file name.

C Change the path shown either manually or use the *Change Path* button.

D Click on the *Save* button to save the spectrum file.

The *Mode* tab allows to set up the output format for the spectrum data to be saved.
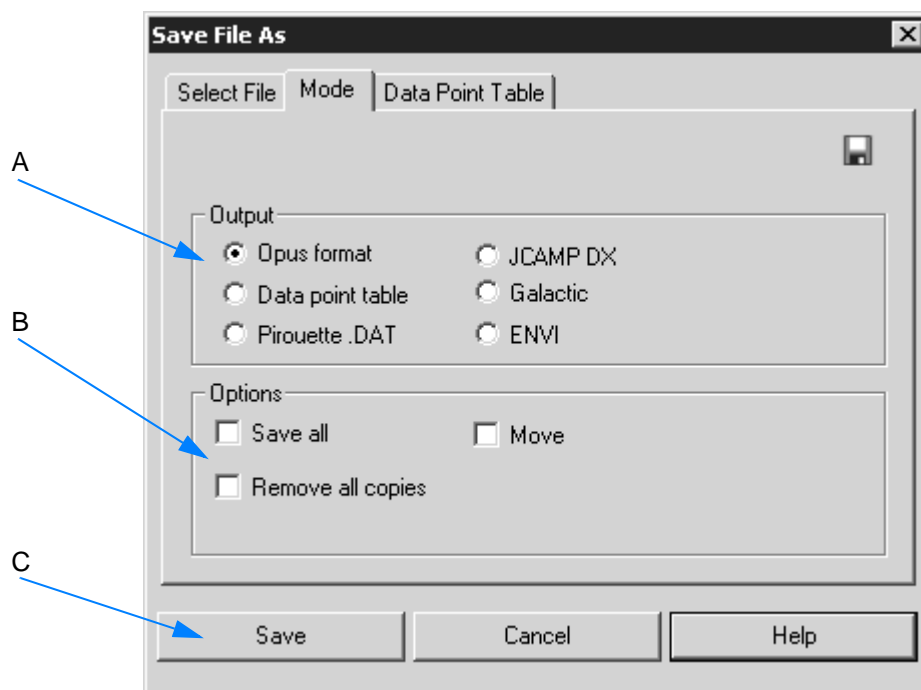
Figure 71: Save File As, Mode

A Output formats available

B Additional saving options available, provided you have checked the *OPUS format* option button first. If you check the *Save all* option button, all data blocks will be saved. You can also move the original spectrum file, or automatically remove all copies of the spectrum file.

C Click on the *Save* button to save the spectrum file.

The *Data Point Table* tab is not available for the OPUS Mentor software package.

3.1.5　Undo Changes ↰

Definition	This command undoes all changes made in a spectrum file since it has been saved for the last time. The original data will be restored, but the History report which includes all the previous manipulations will not be reset.
Principle	Select the spectrum file and click on the *Undo Changes* command. A dialog opens which automatically contains the name of the spectrum file in the *File(s) to undo changes* selection field. Click on the *Undo* button.

3.1.6　Send File 📧

Definition	OPUS spectrum files can also be sent by e-mail
Principle	Select the spectrum file and click on the *Send File* command. A dialog opens which automatically contains the name of the spectrum file in the *File(s) to send* selection field.
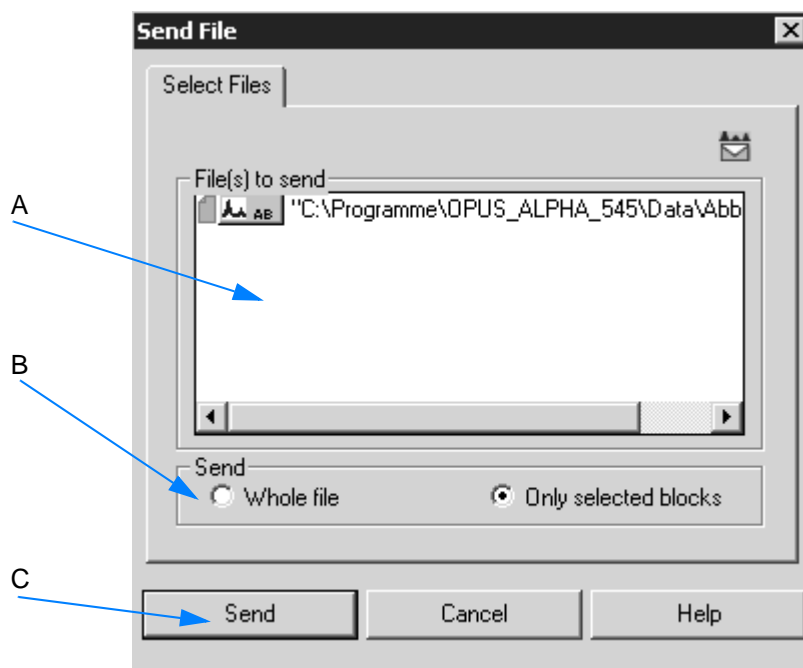
Figure 72: Send File

A The name of the spectrum file is automatically shown in the *File to save* selection field.

B Sending options available to send the whole file or particular data blocks only.

C Clicking on the *Send* button will transfer the data to the Windows mail program. You can specify an address and write a comment. If you use the mail program for the first time, you will automatically be prompted to configure it. The data will be sent as attachment. If the addressee uses an appropriate mail program, it is possible to drag and drop the attachment from this program directly to the OPUS spectrum window.

3.1.7 Clone Entry /Clone Original

Definition	The *Clone Entry* and *Clone Original* commands are used to duplicate spectrum files. The *Clone Entry* command makes a copy of a data file that has been manipulated (e.g. by baseline correction).The *Clone Original* command creates a copy of the original data file (manipulations made will not be stored).
Principle	In either case select the file and click on the respective command. A dialog opens which automatically contains the name of the spectrum file in the *File(s) to clone* selection field. Click on the *Clone* button.
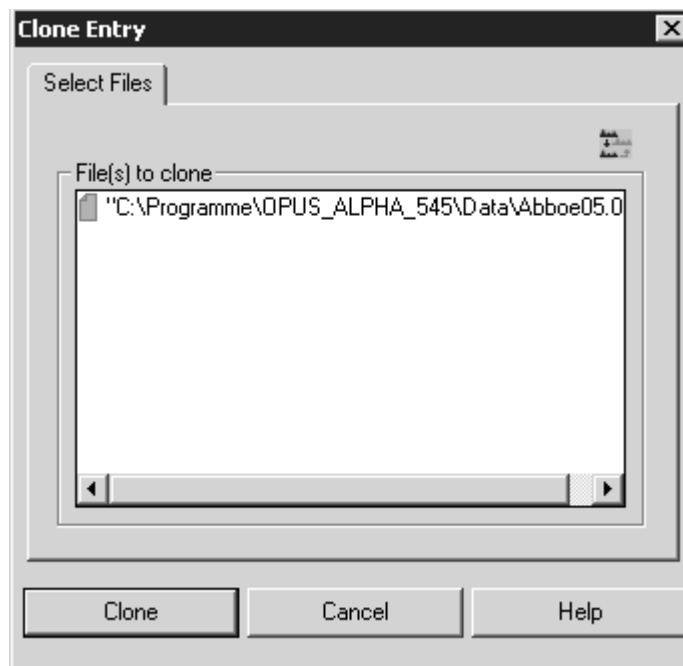
Figure 73: Clone Entry - Select Files tab

Note: When storing the changes made in a cloned file you have to use the *Save File As* command if you do not want the original file to be overwritten by these changes, and use a different file name for the cloned file.

3.1.8   My Work 📖

Definition

The *My Work* command allows to run a lab journal (LabJournal). This automatically-generated lab journal records what kind of evaluations or measurements have been performed in OPUS, how and when. The evaluation and measurement data stored are displayed in a special view.

The lab journal data are sorted by the:
• name of the spectra file
• type of evaluation or measurement
• date

Lab journals are files with the *.lbj* extension, which are stored in the OPUS directory. The lab journal file name contains the name of the user who created the lab journal, and who is assigned to the journal.

When creating a lab journal...

1   ...select the *User Settings* command from the *Setup* menu and click on the *Basic Settings* tab.

2   Activate the *Run a lab journal* check box (A in figure 74) otherwise it will not be possible to create a lab journal.

A
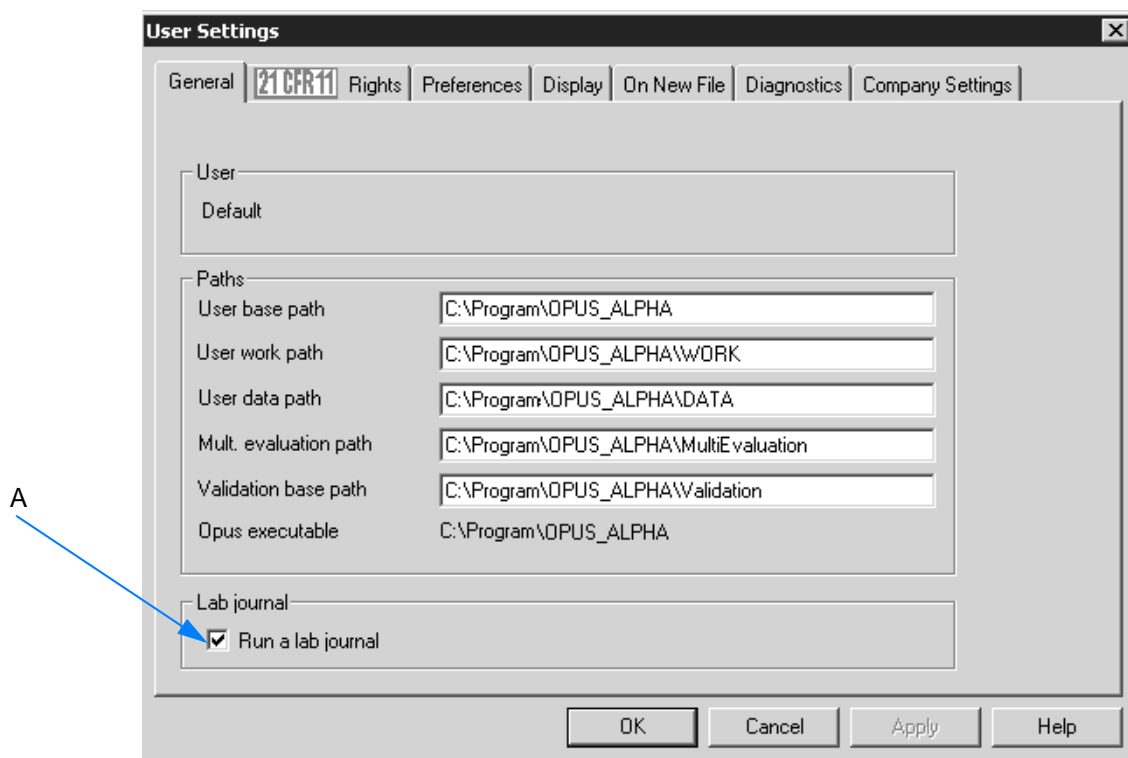
Figure 74: User Settings - Run a lab journal

3   Click on the *My Work* command in the *File* menu. If no lab journal can be assigned to you, you will be asked whether a new journal has to be created. Confirm the dialog that pops up by *Yes*. OPUS automatically creates a lab journal with your user name.

Note: If you have *Administrator* or *Labmanager* user rights, the *Open* dialog will first be displayed. Select the respective lab journal from this dialog.

Depending on the user rights...

...defined (see chapter 1.7) you either have limited or full access to the lab journals in OPUS.

- **Operator:** you can only access the lab journal assigned to your account.
- **Administrator** or **Labmanager:** you can access the lab journals of other users as well.

3.1.8.1 Lab journal view
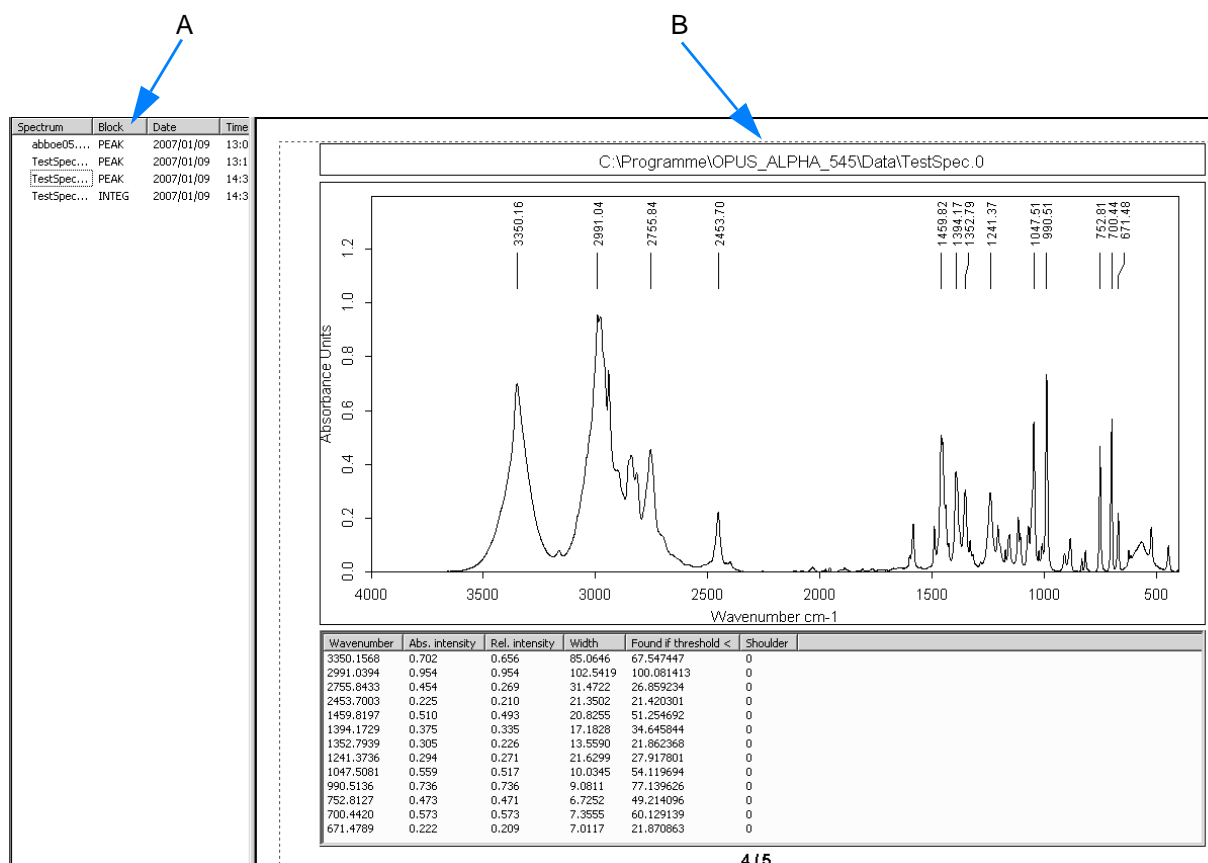
Figure 75: Lab Journal View

A This window shows a list of spectra file names as well as the date of different evaluations or measurements performed. These evaluations or measurements performed are indicated in the *Block* column as follows:

- INTEG: Integration
- PEAK: Peak Picking
- QCMP: Quick Compare
- QUANT: Quantitative analysis
- MEAS: Measurement

Note: The lab journal does not contain all evaluation commands available in OPUS but only the ones mentioned above.

B You can have the evaluation or measurement results displayed on the right side by clicking on the spectra file name.

Double clicking on a spectrum file name opens the spectrum window and displays the spectrum selected, together with the evaluation or measurement results.
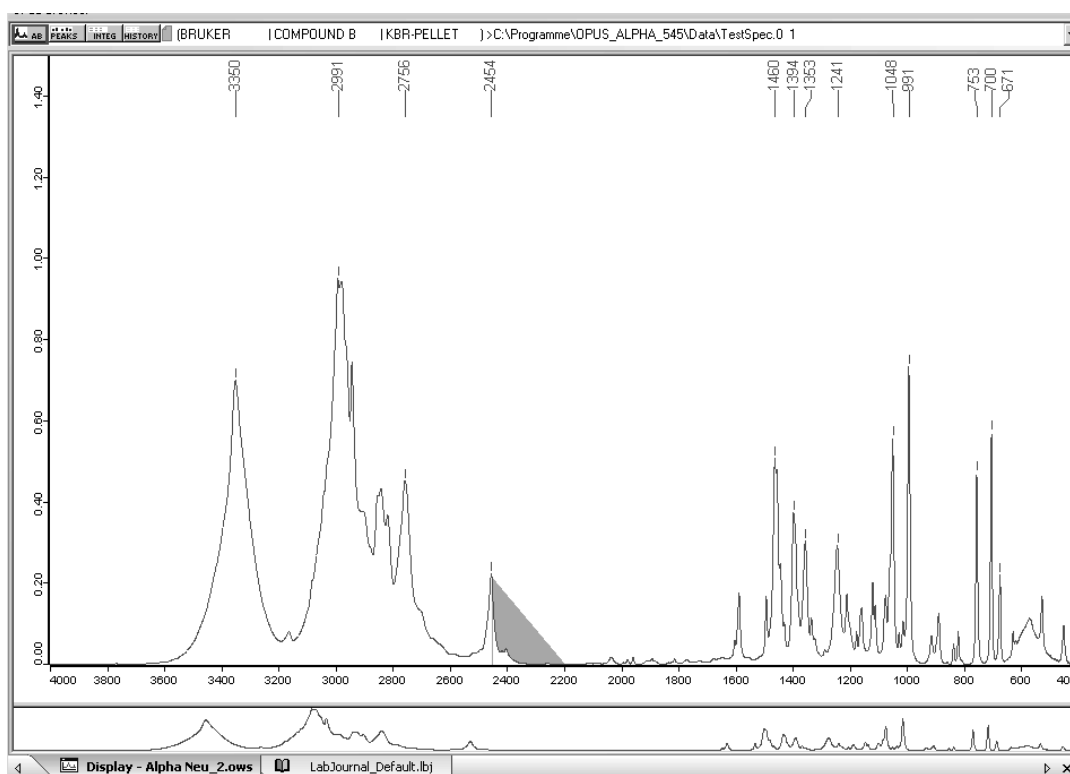
Figure 76: Spectrum window view

Lab journal entries

One single lab journal contains up to 1000 entries. If the number of entries exceeds the limit of 1000, the lab journal will automatically be renamed and copied into a sub-folder for archiving purposes.

When renaming, the date of the first and last entry are added to the previous file name. Thus, the new file name indicates the time period of the different entries. The following format applies to the new file name:

YYYYMMDD: YYYY = year, MM = month, DD = day

Example: *LabJournal_Default_2006-03-15_2006-04-10*

If the previous journal has been archived, OPUS creates a new journal using the *LabJournal_Default.lbj* name.

The lab journal can also be printed with each lab journal entry being on a separate page. Select the *Print* command from the *File* menu.

When sorting lab journal entries...

...in ascending or descending order click on the particular column title.You can sort the lab journal entries displayed on the left according to

- spectra file name
- block
- date

Clicking again on the particular column title restores the original sorting order.

When sorting by date...

...you have the possibility to limit the entries to a certain period of time.

1   Double click on the *Date* column to open the following dialog:
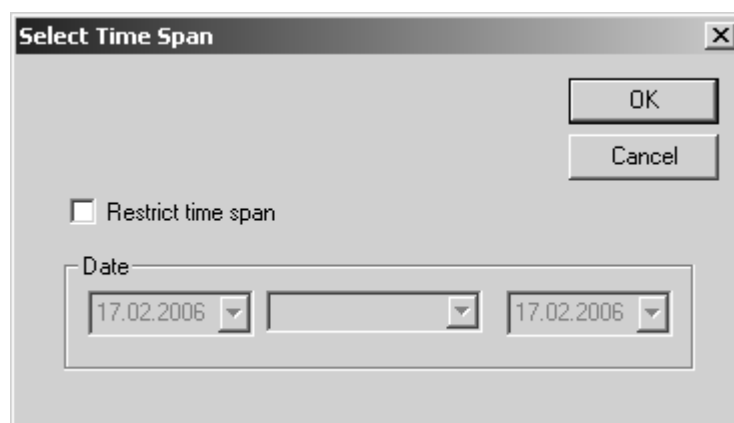
Figure 77: Lab Journal - Select Time Span

2   Activate the *Restrict time span* check box.
3   Determine the period of time using the drop-down lists.
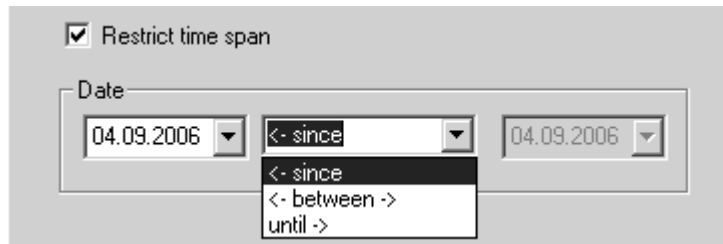
4   Confirm the settings by clicking on the *OK* button. The list will be sorted again, considering only those evaluations or measurements selected within the defined period of time.

5   To undo this setting double click again on the *Date* column. Deactivate the *Restrict time span* check box and click on the *OK* button.

3.1.9   New/Open

Definition	The *New* command allows to select different OPUS views, e.g.: • OPUS • PLE • VBScript • GMacro The *Open* command allows access to the OPUS workspaces available.
Principle	Select the *New* command to open the respective OPUS view. Click on the *Open* command and select the respective workspace from the dialog shown.

3.1.10 Print

Definition	The *Print* command allows printing reports.
Principle	The report data are either printed on the printer or into a different file.

3.1.11 Print Preview

Definition	The *Print Preview* command allows to view several pages of a report in reduced size. **Note: This command is only available if a report window is displayed.**
Principle	If you have selected this command, you can individually edit the report before printing it.

3.1.12 Print Setup

Definition	The *Print Setup* command allows to define printer settings.
Principle	You can define the paper size and print-out format. These settings will be standard for all OPUS print-outs.

3.1.13 Exit

If you select the *Exit* command, the OPUS program will close.

3.2 Edit Menu

The *Edit* menu includes features for information input, options to edit structures as well as the standard Windows commands *Copy* and *Paste*.
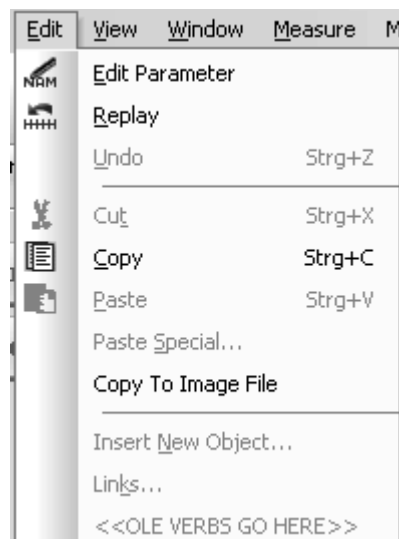
Figure 78: Edit Menu

3.2.1   Edit Parameter ✎

Definition	The *Edit Parameter* command allows to edit the most important sample parameters, e.g. sample name, sample form, operator name and sample number. **Note: When working in GLP mode[1] you will not be able to change these parameters.**
Principle	First, load the spectrum file which parameters you want to edit and select the *Edit Parameter* command. A dialog opens which automatically contains the name of the spectrum file in the *Select file* selection field.

1. GLP = Good Laboratory Practice; regulations for laboratories and producers on how to plan, perform and control tests and measurements.
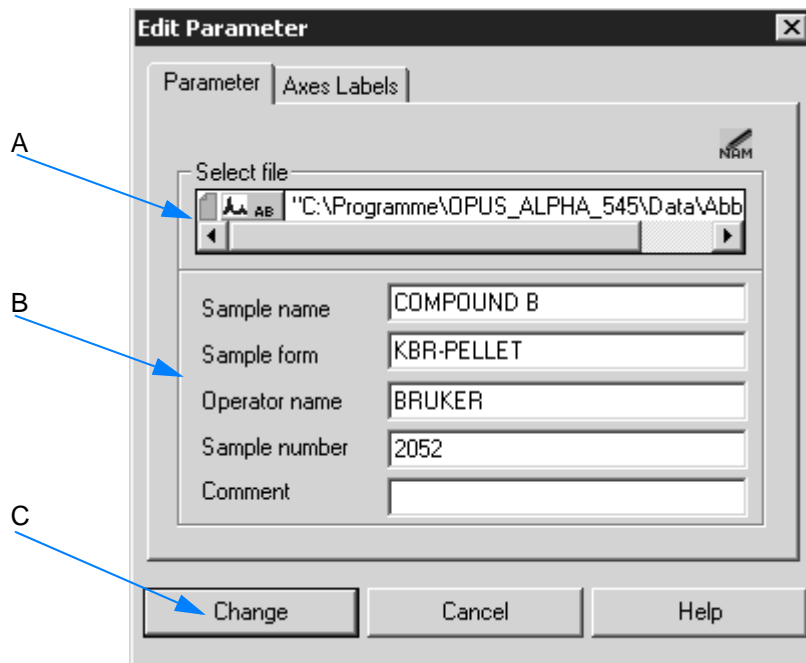
Figure 79: Edit Menu - Edit Parameter

A The name of the spectrum file loaded is automatically shown in the *Select file* selection field.

B Manually enter the changes into the respective entry field.

C Click on the *Change* button to have the changes become effective.

The *Axes Labels* tab allows to edit the axes labeling of the spectra, and set a scaling factor for the axes. The settings made are considered when printing the spectrum file.
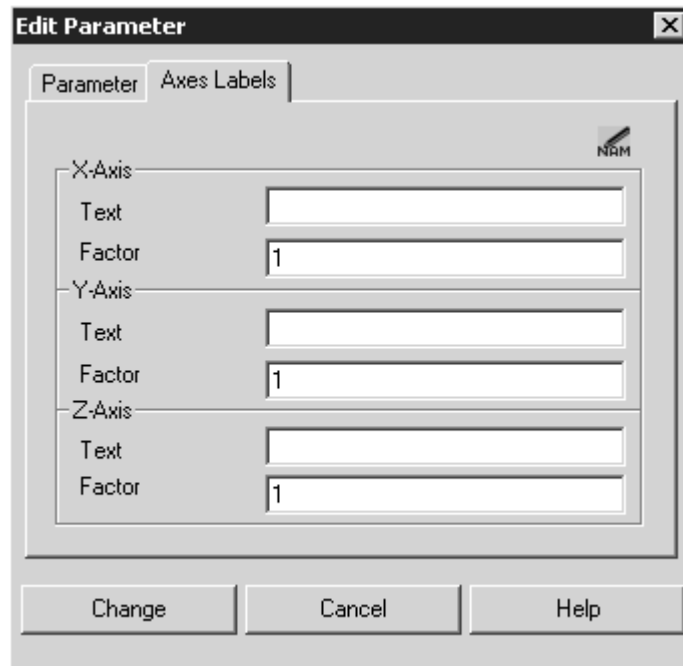
Figure 80: Edit Menu - Edit Parameter, Axes Labels

3.2.2 Replay

Definition	When working in GLP mode[1] a copy of the original spectrum is saved together with the corresponding data. On the basis of this original spectrum, you can repeat some of the manipulations performed.
Principle	First, load the spectrum file and select the *Replay* command. A dialog opens which automatically contains the name of the spectrum file in the *Select file* selection field.

1. GLP = Good Laboratory Practice; regulations for laboratories and producers on how to plan, perform and control tests and measurements.

A

B

C
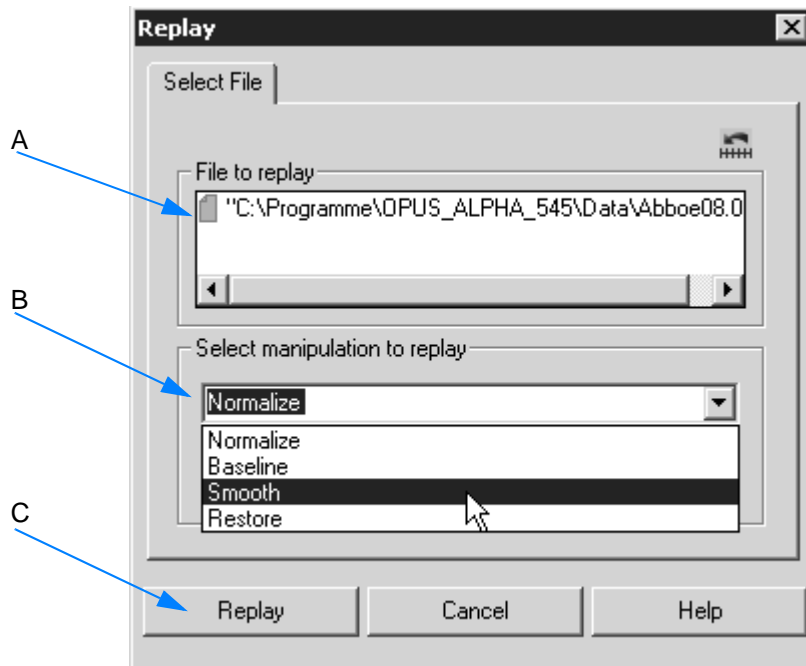
Figure 81: Edit Menu - Edit Parameter

A The name of the spectrum file loaded is automatically shown in the *File to replay* selection field.

B Select the manipulation command from the drop-down list, which you want to repeat. If you select *Smooth*, as exemplified in figure 81, the *Normalize*, *Baseline* and Smooth manipulation commands will be performed on the original spectrum.

3.2.3 Cut ✂

If you cut a selected object, it will be removed and stored in the clipboard.

3.2.4 Copy 📄/Paste 📋

If you copy a selected object, it will be stored in the clipboard. To insert the data of the clipboard into the active file or window click on the *Paste* icon in the toolbar, or select the *Paste* command from the menu.

3.2.5   Copy to Image File

Definition	The command *Copy To Image File* allows to store the current OPUS view as image file, with the following formats being available: • *.bmp (Bitmap) • *.pdf (Portable Data Format) • *.emf (Enhanced Metafile)
Principle	If you select the command, a dialog opens in which you define the file name and path as well as the file format.

3.3   View Menu

The *View* menu allows to configure the OPUS user interface. You can define the toolbars, hide or unhide the status bar, browser or wizard window as well as the permanent report view.
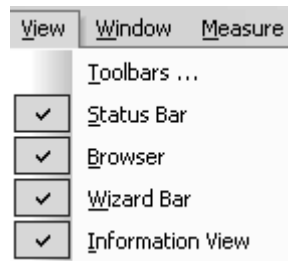
Figure 82: View Menu

3.3.1   Toolbars

Definition	For each OPUS menu a toolbar is available which can be individually customized. Generally, the toolbars include icons of frequently-used commands.
Principle	If you click on the *Toolbars* command, the *Customize* dialog opens. The options provided allow to customize toolbars and configure single icons. For further details on this subject refer to chapter 3.12.5.

3.3.2   Status Bar

Definition	The status bar informs about the background tasks of pro-grams running in OPUS, and displays their current status (see figure 13 on page 17).
Principle	To activate or deactivate the status bar, check or uncheck the *Status Bar* command.

3.3.3   Browser

Definition	The browser contains the spectrum files with the correspond-ing data blocks.
Principle	To activate or deactivate the status bar, check or uncheck the *Browser* command. For further information on the browser refer to chapter 1.11.

3.3.4   Wizard Bar

Definition	The OPUS wizard is an interactive help tool which facilitates the measuring of samples, as well as manipulation and evalua-tion of spectra.
Principle	To activate or deactivate the status bar, check or uncheck the *Status Bar* command. For further details on the wizard refer to chapter 1.12.

3.3.5   Information View

Definition	The information view on the lower OPUS interface shows the data parameters, manipulation and evaluation results of a par-ticular spectrum files.
Principle	To activate or deactivate the information view, check or uncheck the *Information View* command. For further details refer to chapter 1.15.

3.4 Window Menu

The *Window* menu allows to open new windows and customize their position and appearance. If you load a file, OPUS automatically opens the appropriate window to this file.
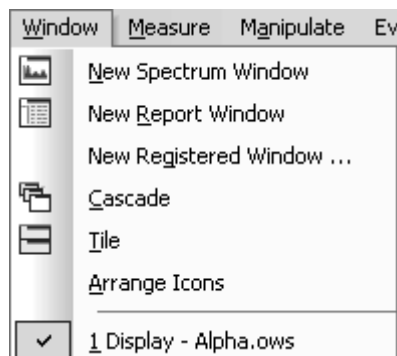
Figure 83: Window menu

3.4.1 New Spectrum Window

Definition	The *New Spectrum Window* command opens a new spectrum window.
Principle	Select the command to open a new spectrum window and load a spectrum file. It is possible to have several spectrum windows open simultaneously.

3.4.2 New Report Window

Definition	The *New Report Window* command opens a new report window. A report window contains data parameters of a spectrum file as well as evaluation results.
Principle	Select the command to open a new report window. Drag and drop the respective data block from the browser in the spectrum window view into the report window view. See also chapter 1.15.2.

3.4.3   New Registered Window

If you click on the *New Registered Window* command, a drop-down list opens which contains all types of OPUS windows available. You can open any type of blank window by selecting the particular window from this list.

Window Name	Definition
CorrelChart	To display a band assignment chart
Display	To display spectra
EvalResults	To display evaluation results
GridReport	GridReport window
OldReport	Shows report in the OPUS format
QCompResult	To display Quick Compare results
Report	To display report blocks
SearchResults	To display the result of a search performed
SingleReport	To display a report without the tree structure
Structure	To display molecular structures generated with a structure editor
Text View	To enter text manually or copy a text file

3.4.4   Cascade

Definition	The *Cascade* command allows to arrange the windows accordingly. The name of the window is shown in the window title bar.
Principle	If you select the *Cascade* command, the windows are automatically cascaded.
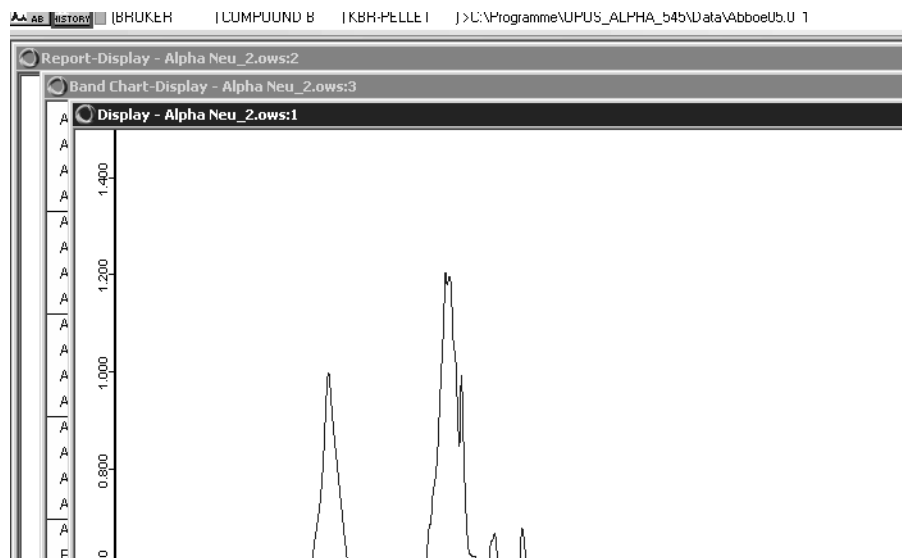
Figure 84: Cascaded windows

3.4.5   Tile

Definition	The *Tile* command allows to arrange the windows accordingly. The windows are reduced and repositioned.
Principle	If you select the *Tile* command, the windows are automatically tiled.
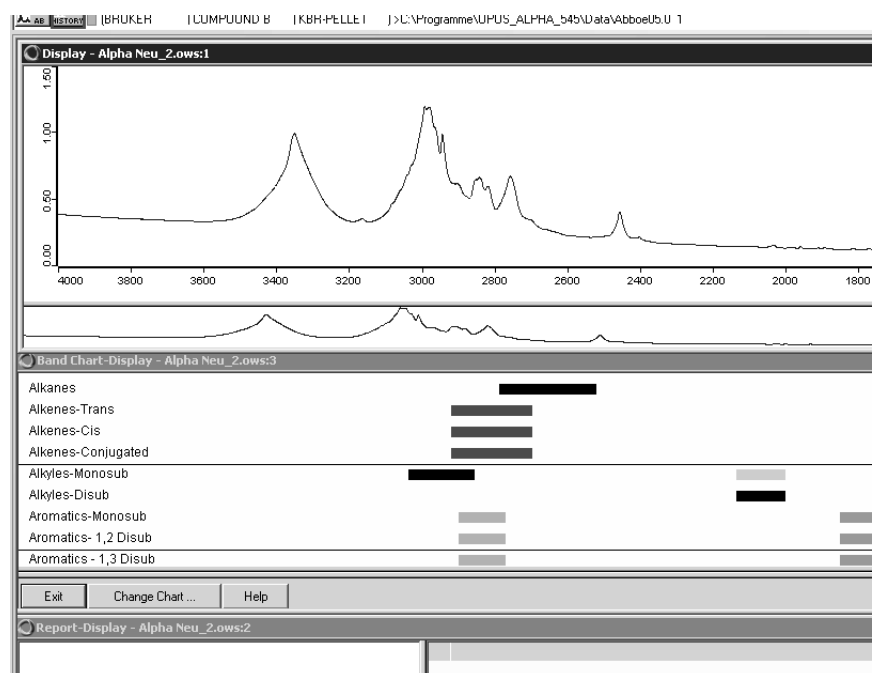
Figure 85: Tiled windows

3.4.6   Arrange Icons

Definition	If you have minimized several spectrum or report windows, they are displayed as small bars. You can have these mini-mized bars re-arranged by drag & drop. By default, the bars are located at the bottom of the OPUS user interface.
Principle	Minimize the windows and select the *Arrange Icons* command.
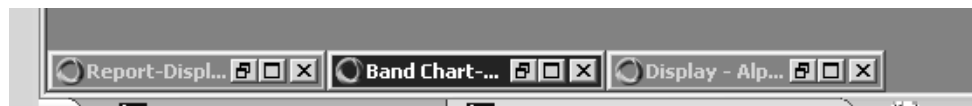
Figure 86: Windows arranged as icons

3.5   Measure Menu

The *Measure* menu allows to start measurements as well as define, save and reload measurement experiments.
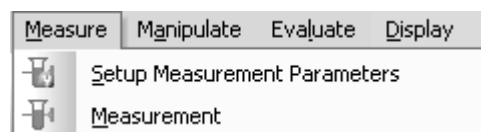
Figure 87: Measure Menu

If OPUS has been started and both the spectrometer status indicator and the OPUS status light are green, you can prepare a measurement experiment with the corresponding parameters.

When starting OPUS next time the parameters used for the last OPUS experiment will be loaded by default. If this is exactly the experiment you want to use, just continue, otherwise you will have to prepare a new experiment with different parameters.

Different default measurement experiments are available in OPUS. The files for these experiments are stored in *C:\Program\OPUS\XPM*.

3.5.1   Setup Measurement Parameters

Definition	The *Setup Measurement Parameters* command allows to set up, edit and load parameters for a measurement experiment.
Principle	Each tab of this command contains different setup features. Define these features and save them. By clicking on the *Exit* button all parameter settings made are saved, except for the interferogram peak position. The peak position has to be saved separately by clicking on the *Check Signal* tab (see figure 94). If you click on the *Cancel* button, you exit the dialog box without saving the changes made.
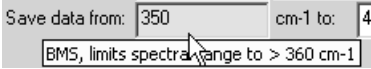
Configuration errors are...

...are indicated by colored entry fields, and warning symbols on the particular tab. Errors during measurement may be caused by:

• The experiment loaded is not compatible with the spectrometer configuration.

• A parameter value is beyond the allowed limit.

The warning symbols and their meaning are described in the following table:

Symbol	Meaning	What has to be done?
⊖	The measurement parameters do not fit with the existing hardware. **No measurement possible!** The entry field of the measurement parameter is marked in red in this case.	• Position the cursor on the red entry field. An error message pops up. • Select one option suggested by OPUS from the drop-down list.
⚠	The value of a measurement parameter is beyond the limits. **No measurement possible!** The entry field of the measurement parameter is marked in red in this case.	• Position the cursor on the red entry field. A help text pops up indicating the cause of the error. Resolution: 1 cm-1 le s Resolution should be greater than 2 • Enter an appropriate value.

Symbol	Meaning	What has to be done?
![i]	The value of an experiment measurement parameter has been changed. **Measurement possible!** The entry field of the measurement parameter is marked in yellow in this case.	• Position the cursor on the yellow entry field. A help text pops up indicating the cause of the error. Save data from: 350 cm-1 to: 4 BMS, limits spectral range to > 360 cm-1 • Enter an appropriate value.
![x]	One measurement parameter is wrong and cannot be corrected. **No measurement possible!** A warning symbol is shown if the experiment contains a wrong parameter, and if the operator is not allowed to change parameters of a measurement experiment.	• Either create a new measurement experiment or • change the user settings accordingly (see chapter 3.12.7).

3.5.1.1 Basic
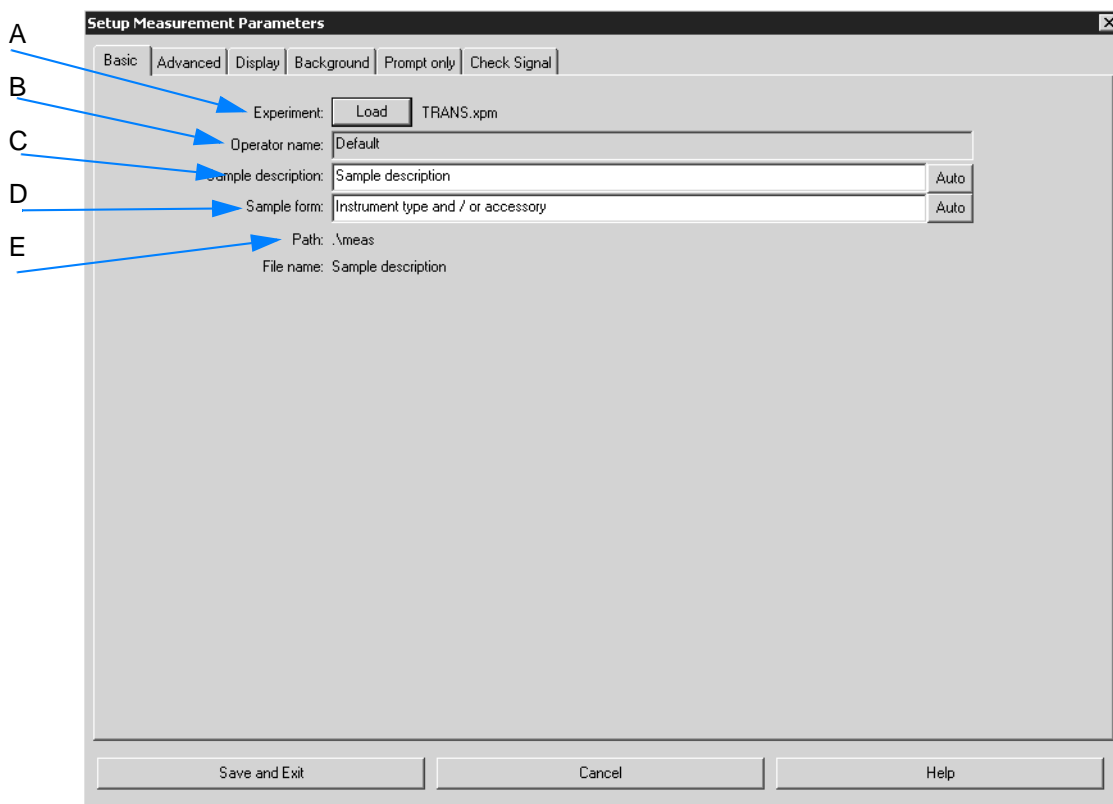
Figure 88: Setup Measurement Parameters - Basic

A   Click on the *Load* button to load an already existing measurement experiment. A dialog opens which you select the respective experiment from.

B   Shows the OPUS operator name logged in.

C   Define the sample name either manually or use automated parameters by clicking on the *Auto* button. For details see below.

D   Define the sample form either manually or use automated parameters by clicking on the *Auto* button. For details see below.

E   Shows the path in which the experiment is stored.

To work with automated parameters...

1   ...click on the *Auto* button (see figure 88) to open the following dialog:
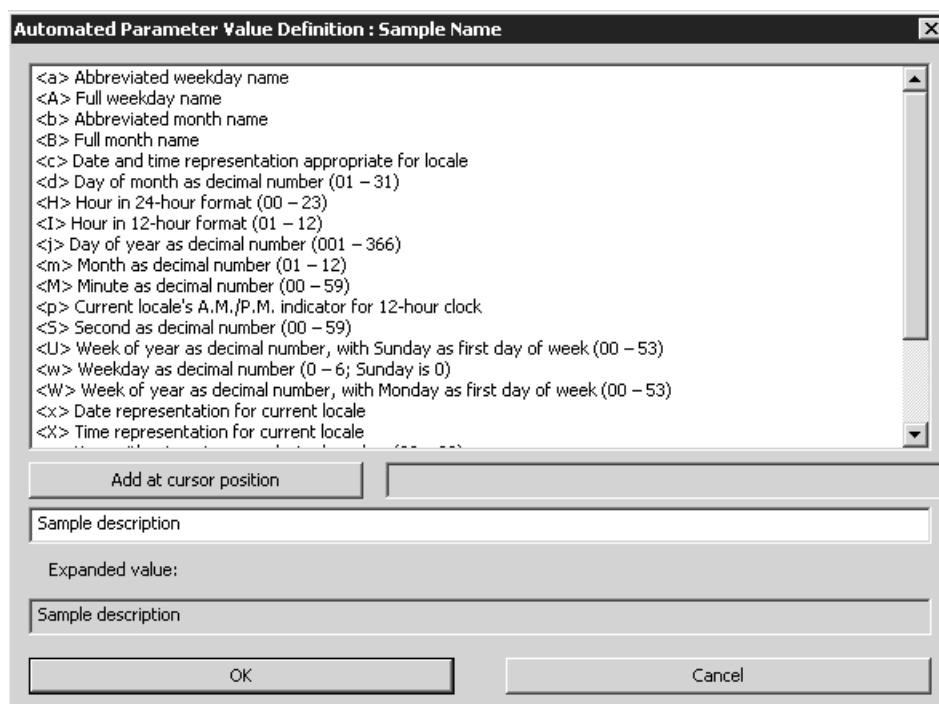
Figure 89: Automated parameters

Note: The list always includes the same automated parameters, whether you define the sample name, sample form or path.

2   Select the parameter desired.
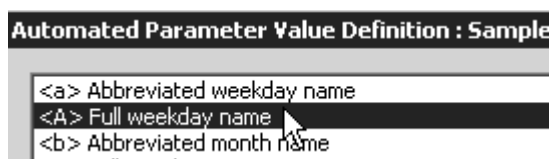
3   The parameter selected is shown in full below the list.
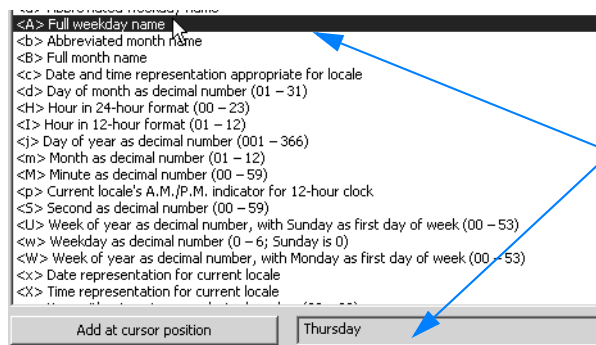
4   First, position the cursor into the entry field and then click on the *Add at cursor position button*. The entry field contains the parameter in pointed brackets. Below the expanded value is shown in full.
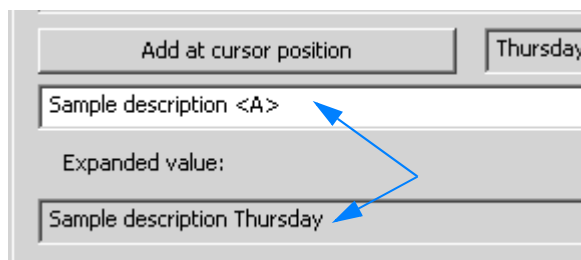
5   You can add several parameters, one behind the other, to one single sample name or sample form. In this case proceed as described above.
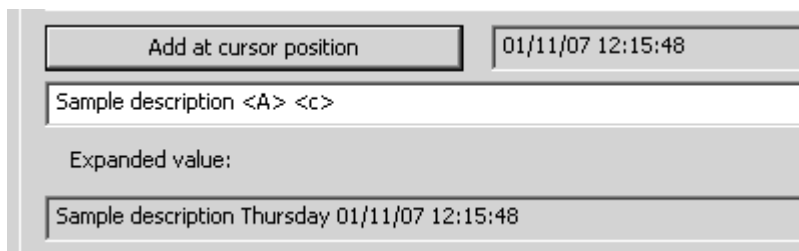
6   To save the settings made click on the *OK* button.

3.5.1.2 Advanced
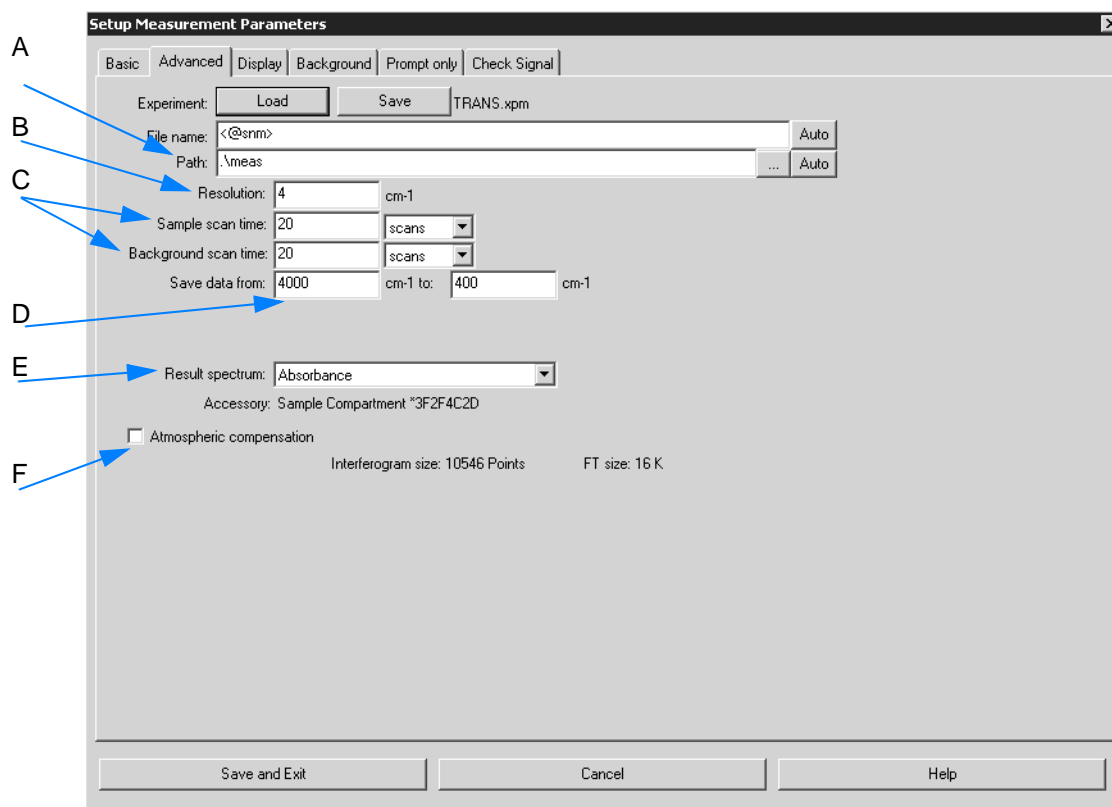
Figure 90: Setup Measurement Parameters - Advanced

A Define the directory path either manually or by clicking on the ⌐ button. To add automated parameters click on the *Auto* button.

B Define the resolution. **Tip: Make sure not to set the resolution higher than necessary to minimize the total acquisition time. Improving the resolution, e.g. by a factor of 2, requires a four-times higher acquisition time at a constant signal-to-noise ratio of the spectrum. This is due to the fact that the signal-to-noise ratio is proportional to the square root of the acquisition time.**

C Define the number of scans for the sample and background measurement.

D Define the wavenumber range to be measured.

E Select one of the following result spectra included in the drop-down list:
- Transmittance
- Absorbance
- Kubelka Munk
- Reflectance
- Log Reflectance
- ATR Spectrum
- PAS Spectrum

F Activate the check box if atmospheric compensation is desired. If the sample measurement has been successful, atmospheric compensation will immediately be performed after the measurement. For details on atmospheric compensation refer to chapter 3.6.11.

3.5.1.3 Display
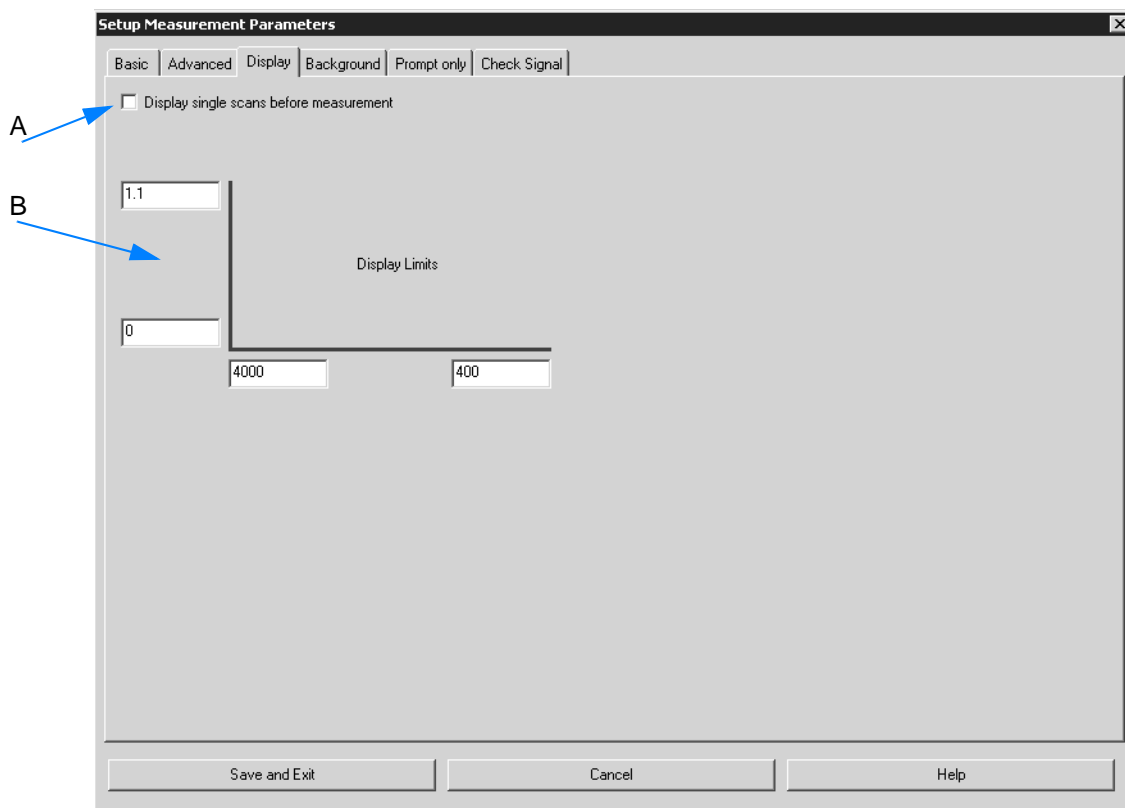
Figure 91: Setup Measurement Parameters - Display

A If you activate the *Display single scans before measurement* check box, the spectrum will be calculated by single scans and displayed, before the actual data acquisition starts. The actual data acquisition is performed as soon as the operator starts measurement.

B Defines the axes settings for the spectrum display during measurement. It is possible to enter upper and lower limits for the x- and y-axis.

3.5.1.4 Background
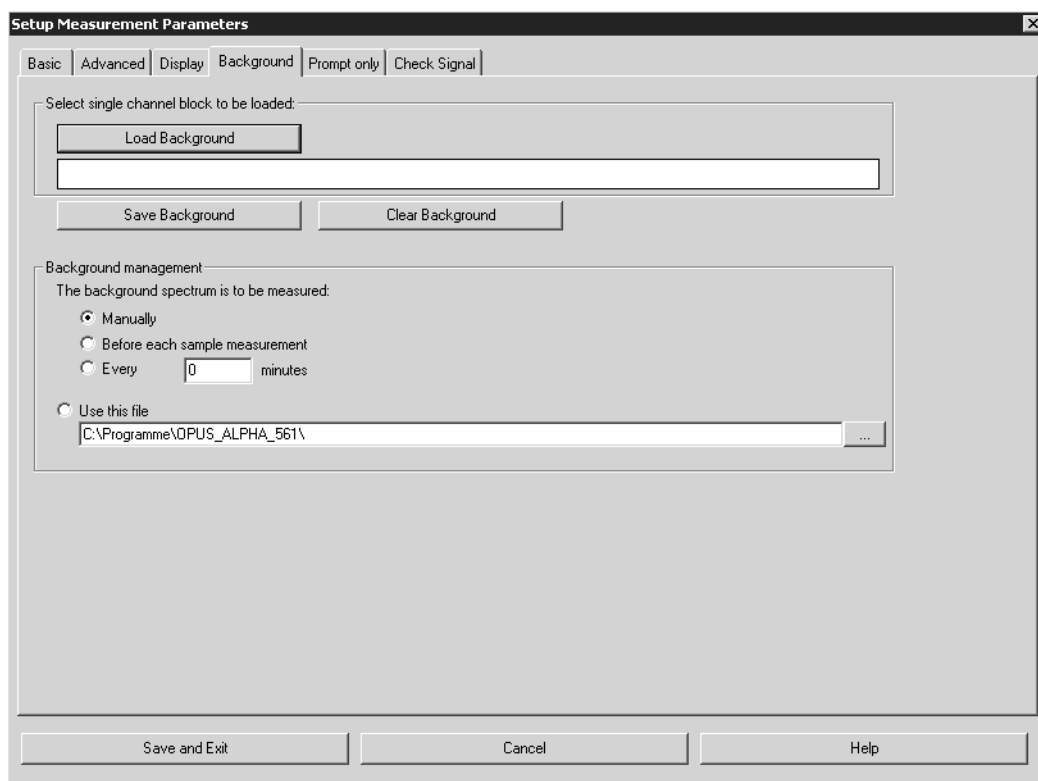
Figure 92: Setup Measurement Parameters - Background

On the *Background* tab you specify the background spectrum and define the reiteration mode of the background measurement.

> **Note: In case of a background measurement no sample is available in the sample compartment or on the ATR crystal. Before performing any sample measurement you first have to perform a background measurement.**

It is recommended to acquire a new background spectrum at the beginning of a new measurement series or after a certain validity period has expired.

A Load a background spectrum by using this button. The name and path of the spectrum file will be displayed in the small field below.

B Define the reiteration mode of the background measurement by activating the respective option button.

3.5.1.5 Prompt only
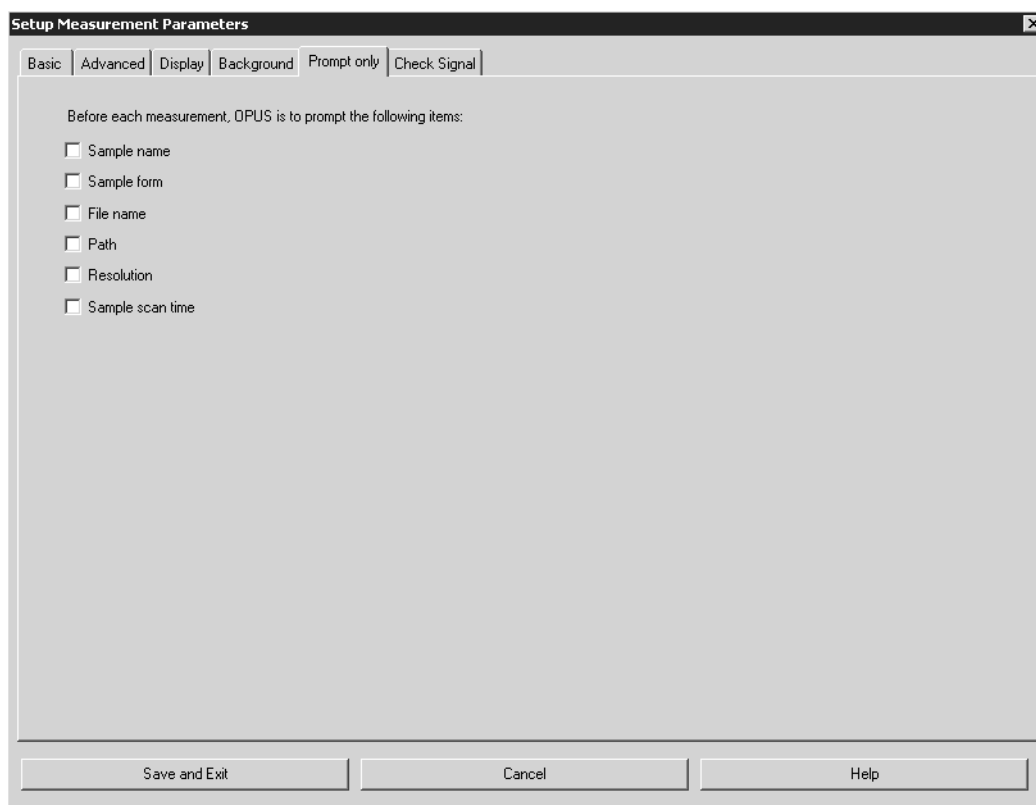
Figure 93: Setup Measurement Parameters - Prompt only

Activate those parameters which OPUS always has to prompt before each measurement.

The parameters defined will be displayed before each measurement in the form of entry fields on the *Measurement* dialog (see chapter 3.5.2). If a particular parameter has to be changed, e.g. file name, click into the respective entry field in the *Measurement* dialog and enter the new name.

3.5.1.6 Check Signal

To determine and save the exact interferogram peak position you have to open the *Check Signal* tab at least once after you have installed your spectrometer.

The purpose of checking the signal is to either achieve a maximum interferogram signal or optimize the shape of the single-channel spectrum.

To zoom into a specific signal range...

1　...right click into the interferogram display and select the *Zoom In* option.

2　A crosshair appears.

3　Press the left mouse button and draw a frame around the signal range.

4　Click on the left mouse button to reposition the frame.

5　Click on the left mouse button again to resize the signal range to the interferogram display.

6　Click on the left mouse button to remove the crosshair.

To zoom out a specific signal range...

1　...right click into the interferogram display and select the *Zoom Out* option.

2　A crosshair appears.

3　Perform the same steps as described for the *Zoom out* procedure.
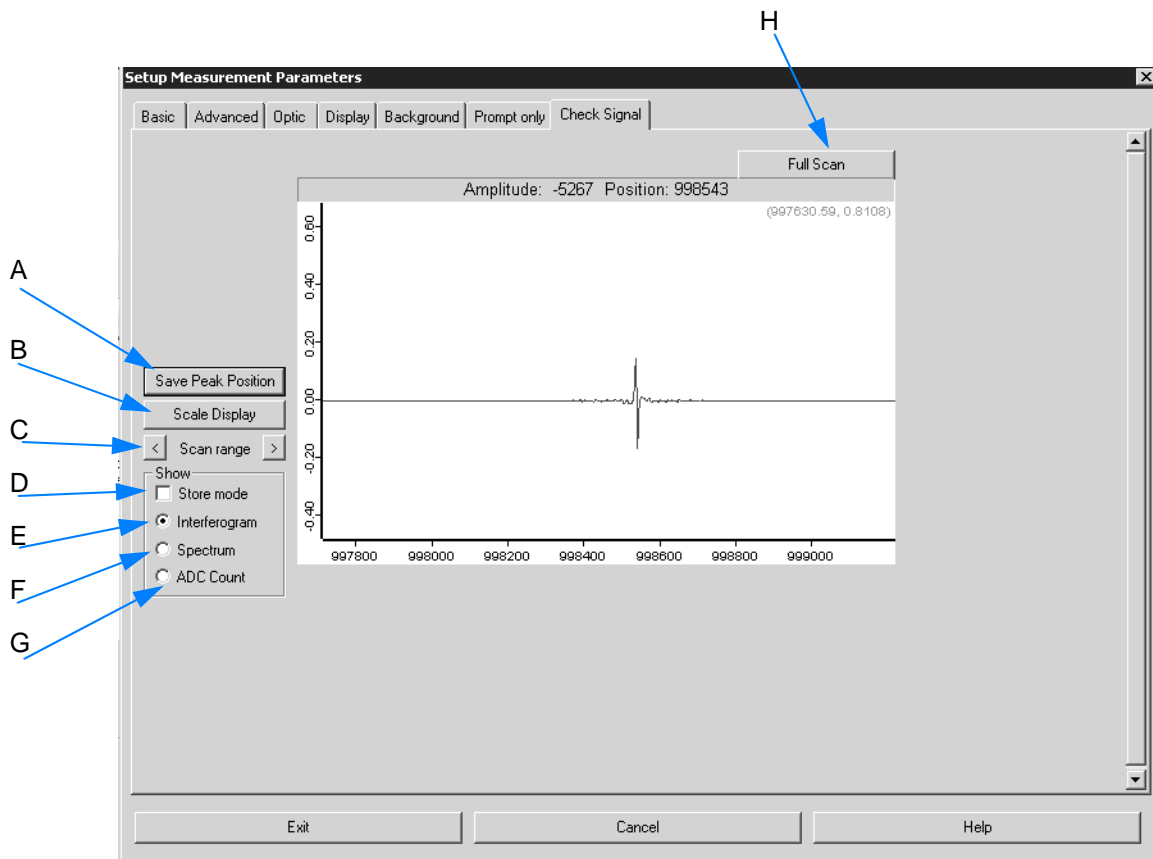
Figure 94: Setup Measurement Parameters - Check Signal

A If the peak position is constant, save it by clicking on the *Save Peak Position* button.

B To undo a former signal range zooming click on the *Scale Display* button, and the interferogram will be scaled on the intensity axis.
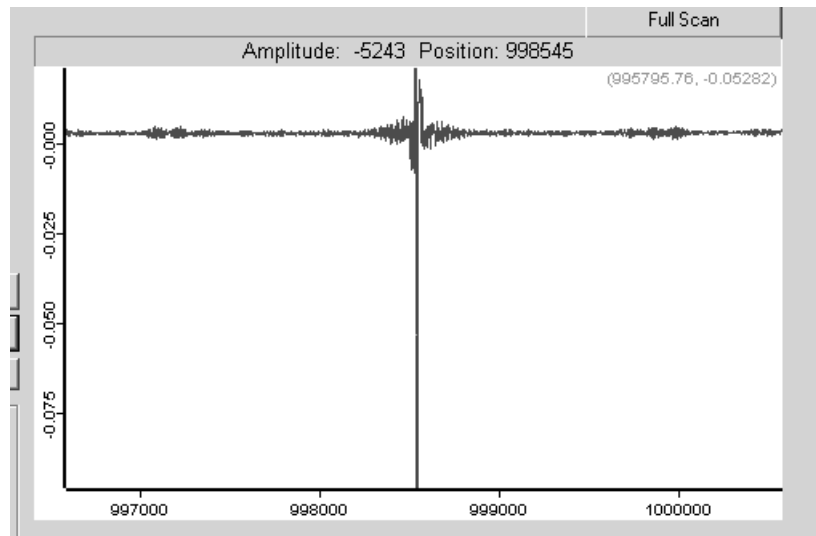
Figure 95: Interferogram scaled on the intensity axis

C If the maximum interferogram value is not displayed, move the range by clicking on the arrow buttons.

D Activate the check box if the display mode should be stored.

E If the option button is checked, the interferogram will be displayed graphically.

F If the option button is checked, the interferogram is Fourier transformed during adjustment and displayed as single-channel spectrum.

G If the option button is checked, the amplitude and zero-crossing position are displayed.
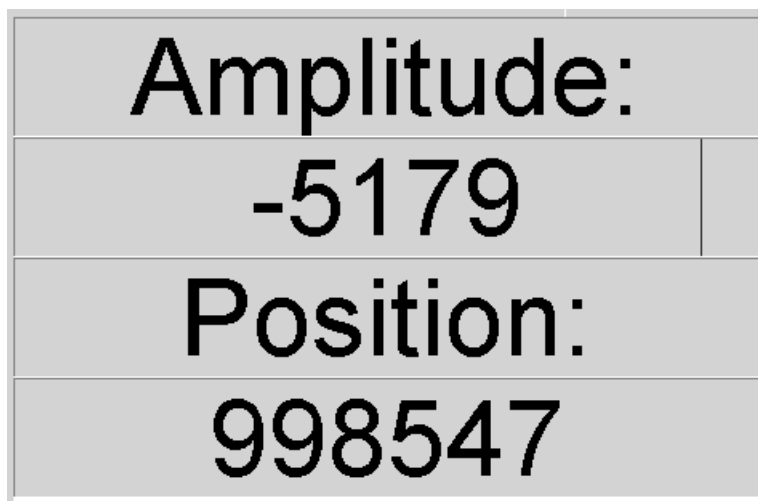
Figure 96: Numerical display of ADC count

H To have the complete scan displayed click on this button.

3.5.2 Measurement

Definition	The *Measurement* command allows to start background and sample measurement.
Principle	Select the command and click on the respective measurement button. **Note: If you start OPUS, the parameters defined for the last OPUS measurement will be loaded by default. If these are not the parameters you want to use, you have to load or create a different experiment. If the measurement has been finished, the parameters will automatically be stored together with the results.**

When do you perform which measurement?

1 Background measurement (reference measurement)

A background measurement is performed without any sample in the sample compartment (transmission) or on the crystal (ATR). This kind of measurement is also called reference measurement. **A background measurement is always to be performed before a sample measurement.** For further information on the background measurement refer to chapter 2.1.

2 Sample measurement

During sample measurement a sample is measured which has been positioned into the sample compartment (transmission) or on the crystal (ATR). **A sample measurement is always to be performed after a background measurement.** In case of a

measurement series, however, it is not necessary to always per-
form a background measurement before each single sample
measurement. For further information on the sample measure-
ment refer to chapter 2.1.

A

B
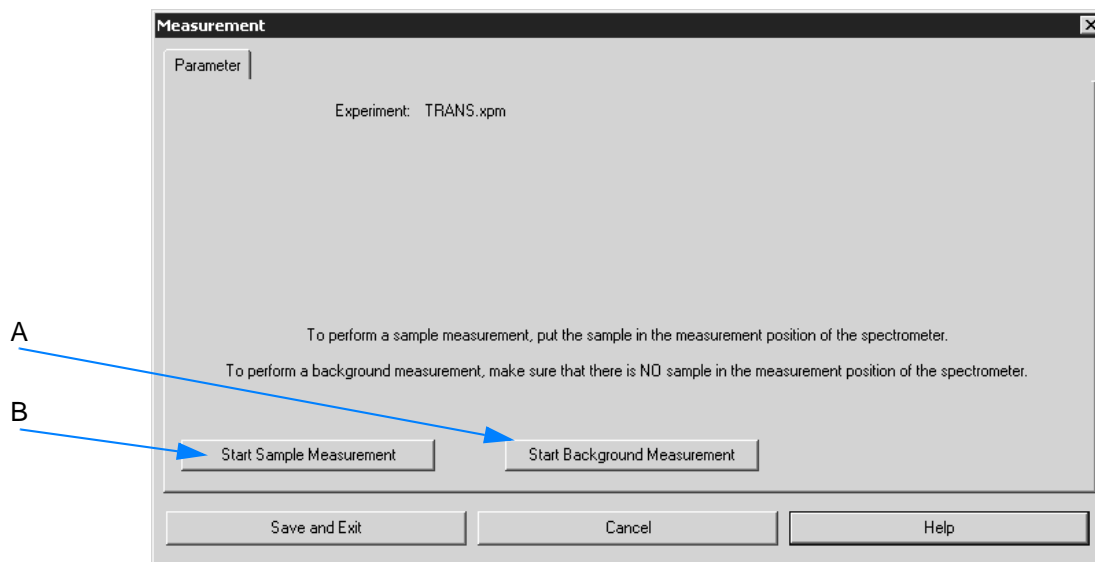
Figure 97: Measurement

A First, start a background measurement.

B Afterwards start a sample measurement.

If the measurement runs...

...the progress is indicated by the status bar at the bottom of the OPUS
workspace and directly below the spectrum window.
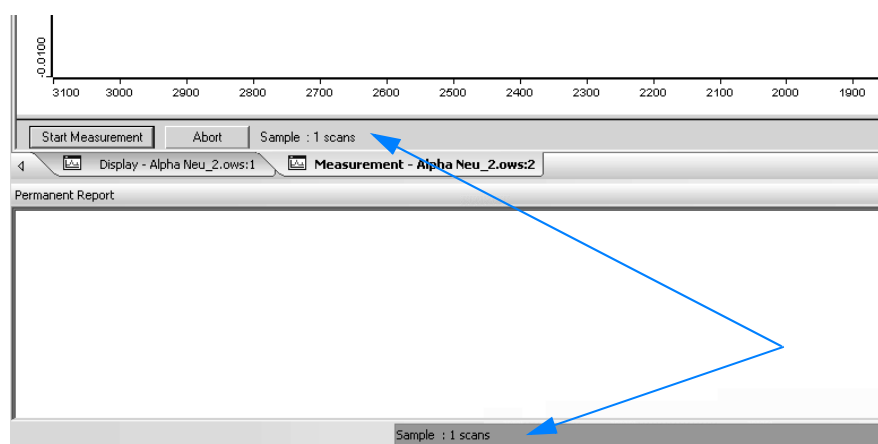
Figure 98: Measurement progress

Right clicking on this status bar opens a pop-up menu which you can use to abort the measurement.
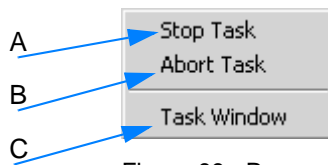
Figure 99: Pop-up menu to stop tasks

    A A running measurement is interrupted (a repeated measurement will be continued by the next spectrum).

    B A repeated measurement is completely aborted.

    C If you click on the *Task Window* command, an additional menu pops up including the current OPUS tasks running.
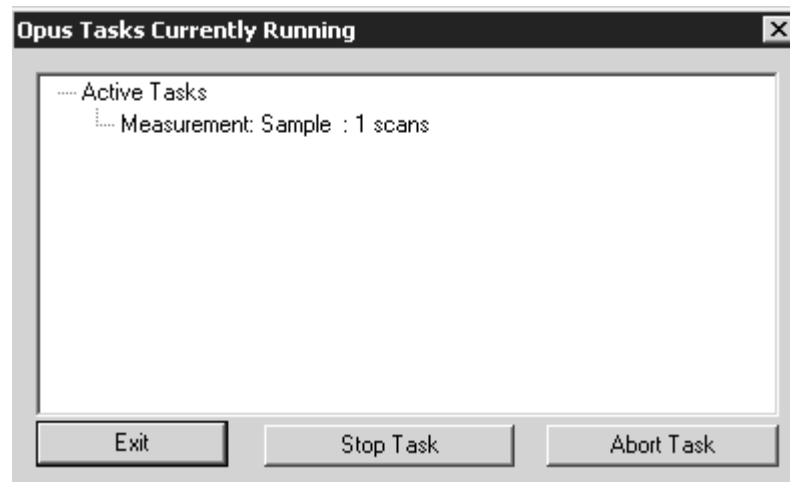
Figure 100: Task window

Select one task from the list and click on the *Stop Task* or *Abort Task* button. If the measurement has been completed, the *No Active Task* message is displayed in the status bar.

3.5.3   Cleanness Test Setup

Definition	This command is only relevant if you work with an ATR measurement module. Use this command to perform a reference measurement of the ATR crystal and define the maximum allowed limit of the crystal contamination.
Principle	Select the command. The dialog displayed in figure 101 opens. **Note: If the *Cleanness Test Setup* command is not available in the *Measure* menu...** •...click on the *Customize* menu command in the *Setup* menu. • Click on the *Commands* tab in the *Customize* dialog displayed. • Select the *Measure* menu from the *Categories* list box. • Select the *Cleanness Test Setup* command from the *Commands* list box. • Drag & drop the command to the *Measure* menu, while pressing the left mouse button. For further information on customizing menus refer to chapter 3.12.

Figure 101: Cleanness Test Setup

1   Perform a reference measurement by clicking on the *Reference Measurement* button. **When measuring make sure that the ATR crystal is not contaminated.**

2 If the reference measurement runs, it will be indicated as follows.
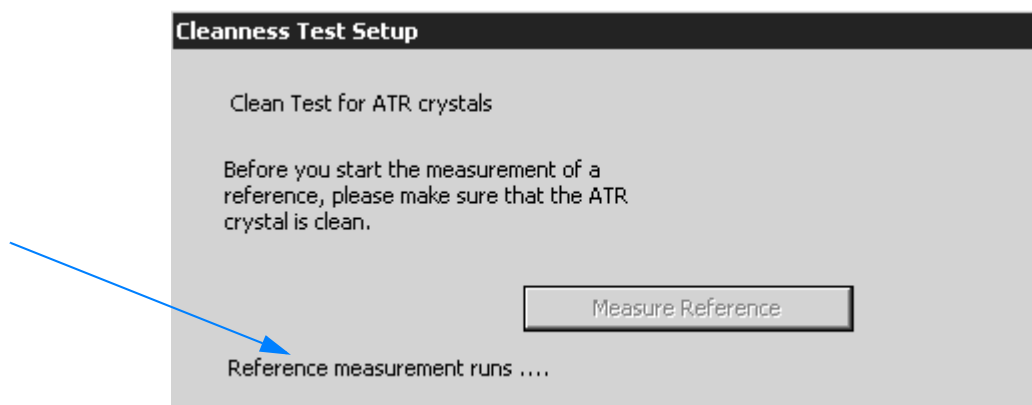
3 If the reference measurement has been finished, the reference spectrum is stored.

4 Define the maximum allowed contamination level. Enter the corresponding value into the entry field.
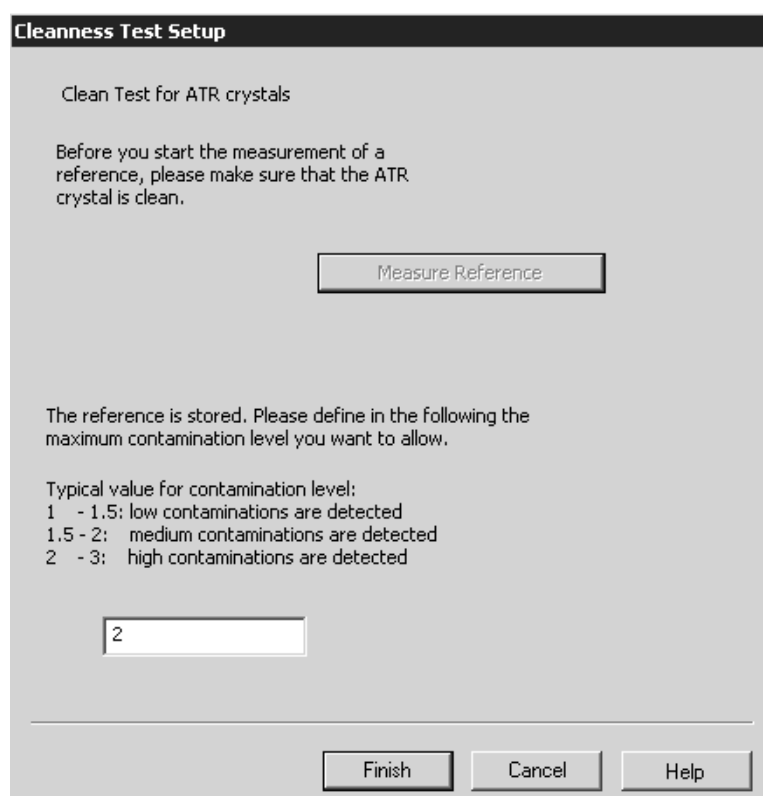
Figure 102: Defining contamination level

5 Click on the *Finish* button.

3.5.4   Cleanness Test 🖳

Definition	Based on the maximum contamination level defined the cleanness test checks whether the ATR crystal is clean. The wave number range is between 2800 and 3050cm^{-1} (absorption).
Principle	Select the command to perform the cleanness test. **Make sure that the ATR crystal does not contain any contaminations.** The dialog displayed in figure 103 opens. **Note: If the *Cleanness Test* command is not available in the *Measure* menu...** • ...click on the *Customize* menu command in the *Setup* menu. • Click on the *Commands* tab in the *Customize* dialog displayed. • Select the *Measure* menu from the *Categories* list box. • Select the *Cleanness Test* command from the *Commands* list box. • Drag & drop the command to the *Measure* menu, while pressing the left mouse button. For further information on customizing menus refer to chapter 3.12.
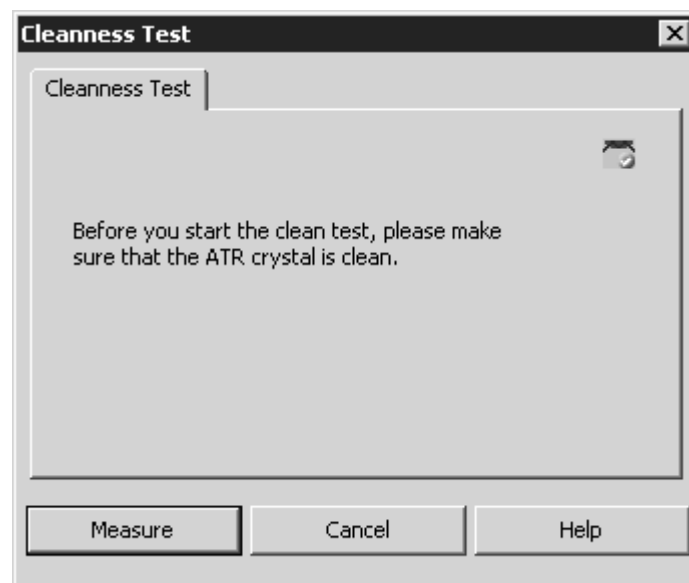
Figure 103: Cleanness Test

To start the cleanness test click on the *Measure* button. The test result is indicated as follows:

• Blue exclamation mark: crystal is clean, i.e. the defined maximum contamination level has not been exceeded

• Red cross: crystal is contaminated, i.e. the defined maximum contamination level has been exceeded
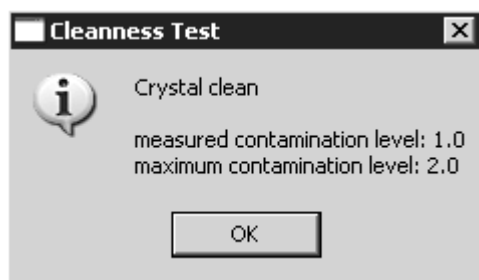
Figure 104: Clean crystal

The contamination level measured is displayed and compared with the maximum allowed level.

If the crystal is contaminated, you can repeat the cleanness test by clicking on the *Repeat* button.
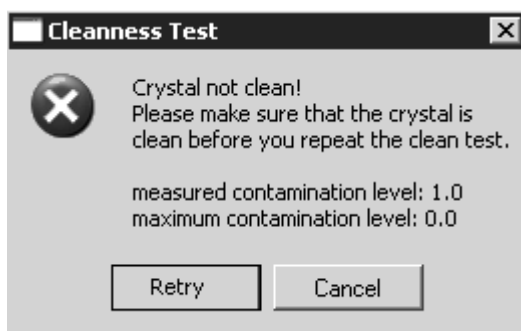
Figure 105: Contaminated crystal

3.6   Manipulate Menu

The *Manipulate* chapter describes the OPUS data manipulation options. In this particular case the term *Manipulate* involves all arithmetic methods which modify or create new spectral data of a spectrum acquired.

Figure 106: Manipulate menu

3.6.1   Baseline Correction

Definition	If the spectrum baseline is not at 0, a baseline correction can be advisable.
	Note: A baseline correction is to be performed if the spectrum baseline deviates too much from a theoretical horizontal line, which may be due to sample scattering losses.
Principle	This kind of correction subtracts baselines from spectra, which allows to get spectra with band edges of up to the theoretical baseline. In case of absorption spectra this corresponds to a theoretical baseline of 0 and of 100% in case of transmission spectra.

For information on how to perform a baseline correction refer to chapter 2.1.3.

Figure 107 shows the original spectrum with the calculated baseline and the corrected spectrum.
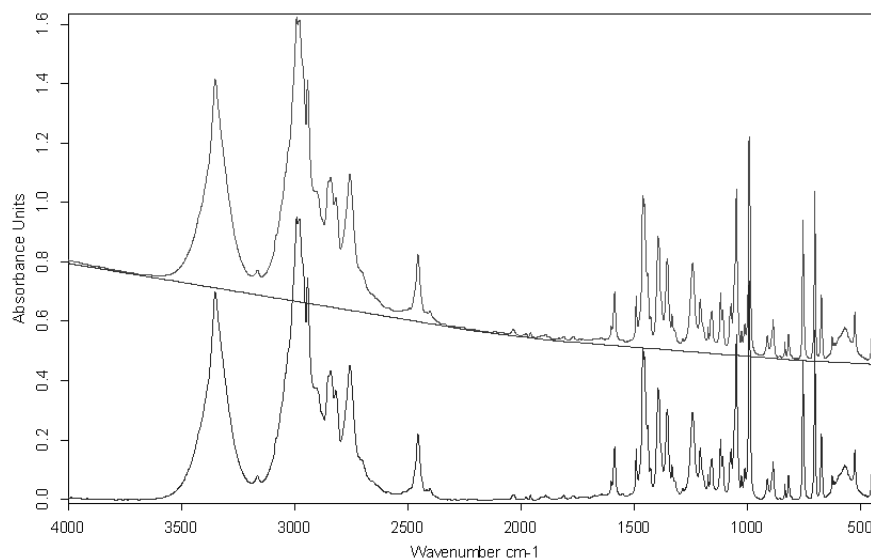
Figure 107: Top: original spectrum and baseline; Bottom: corrected spectrum

3.6.2   Spectrum Subtraction

Definition	Strictly speaking, the IR spectrum of a mixture is the sum of single spectra. In case of such a multi-component spectrum you can get information about one single component by spectrum subtraction. **Note: The spectra to be manipulated (both multi component and single component) have to be available as absorption spectra.**
Principle	This kind of calculation subtracts spectra, with one multiplication factor each, from a multi-component spectrum. An additive constant can be determined. **Note: Transmission spectra are automatically converted to absorption spectra during calculation. Only if the original spectrum has been of transmission mode, the resulting spectrum will be converted to transmission when the subtraction has been finished.**

The subtraction spectrum results as follows:

Subtraction spectrum = (Mixture spectrum - subtraction factor) x Single component

Note: The optimum result can only be achieved if all single components are simultaneously subtracted from one mixture spectrum. This yields to a result of almost 0.

Figures 108 and 109 show the *Spectrum Subtraction* dialogs.
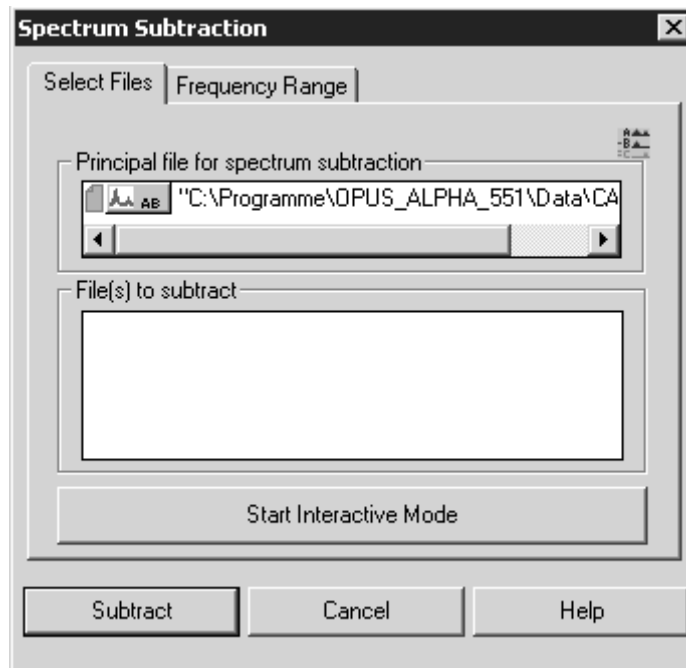
Figure 108: Spectrum Subtraction - Select Files
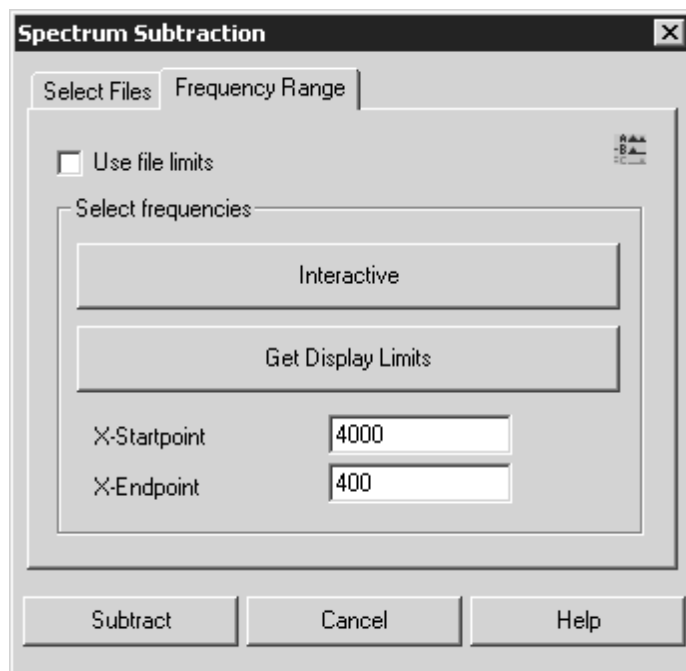
Figure 109: Spectrum Subtraction - Frequency Range

Exemplified spectrum subtraction

1 First, generate an example spectrum using the spectrum calculator (see chapter 3.6.4). The spectrum has to consist of:

- 0.7 parts of the *ABBOE12.0* spectrum parts
- 1.3 parts of the ABBOE08.0 spectrum
- 2.3 parts of the ABBOE05.0 spectrum parts

Note: The spectra are stored in C:\Program\DATA.

2 Save the spectrum as *CALC.6.* This spectrum should represent a generic sample consisting of an unknown amount of these three components.

3 Select the *Spectrum Subtraction* command.

4 Click on the *Start Interactive Mode* button on the *Select Files* tab. The following view is displayed which shows the name of the multi-component spectrum in (A).
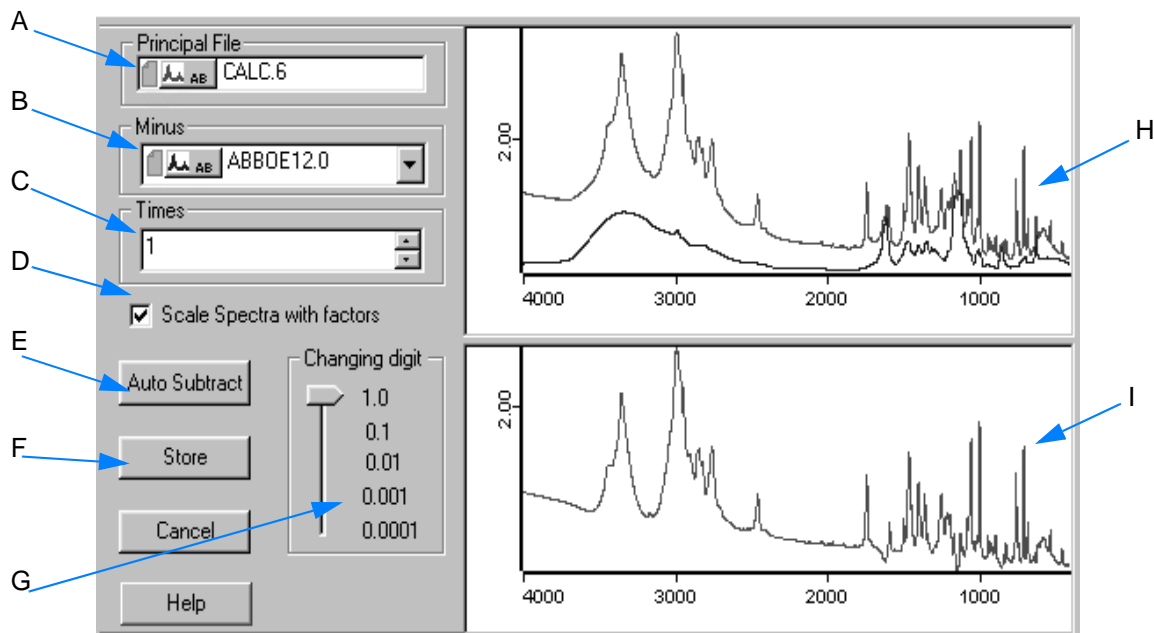
Figure 110: Interactive spectrum subtraction

5 Select the spectra to be subtracted from the drop-down list (B in figure 110).

6 Depending on the spectra selected in (B), the adjusted factors are displayed in (C). The factor value can be increased or decreased, using the arrow buttons on the right. The value can also be entered manually. In this case click into the entry field and over-write the value given.

7 If you activate the check box (D), the displayed spectra will be scaled.

8 Start the automatic spectrum subtraction by clicking on the *Auto Subtract* button (E). **The automatic subtraction mode mini-mizes the least squares deviation in the difference spectrum.**

9   Store the subtraction by clicking on the Store button (F). This will close the view.

By means of the slider (G in figure 110) you define the number of decimals. This causes the factor values of (C) to be adapted.

The window (H) shows both the single-component spectra and the multi-component spectrum. The display in window (I) is autoscaled and shows the difference between the multi-component spectrum and the weighted single-component spectra.
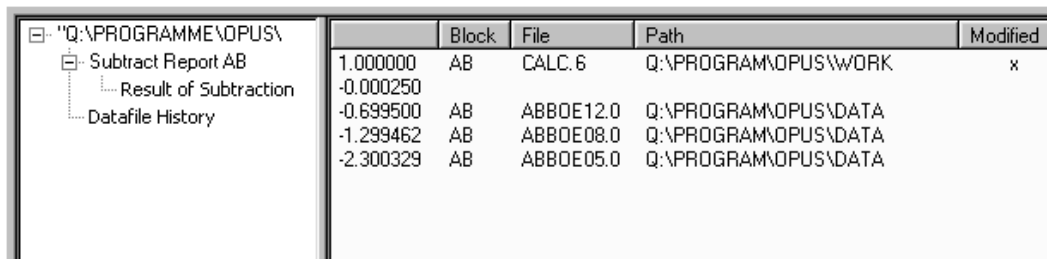
If you right click into the windows (H) and (I), you can zoom in specific spectral ranges using appropriate the option from the pop-up menu.

After spectrum subtraction...

...the numerical values used are attached to the spectrum in the form of a data block.

The subtraction data block contains...

...the factors used to subtract the spectra, as well as the subtraction result spectrum. Double click on the SUBTR data block (𝔰𝔲𝔟𝔱𝔯.) in the browser to open the corresponding report view.

		Block	File	Path	Modified
⊟ "Q:\PROGRAMME\OPUS\	1.000000	AB	CALC.6	Q:\PROGRAM\OPUS\WORK	x
⊟ Subtract Report AB	-0.000250				
⋮ Result of Subtraction	-0.699500	AB	ABBOE12.0	Q:\PROGRAM\OPUS\DATA	
Datafile History	-1.299462	AB	ABBOE08.0	Q:\PROGRAM\OPUS\DATA	
	-2.300329	AB	ABBOE05.0	Q:\PROGRAM\OPUS\DATA	

Figure 111: Spectrum subtraction report

The first column on the right shows the factors and the mark in the *Modified* column indicates the spectrum which the subtraction report has been attached to.

3.6.3   AB <-> TR Conversion ⚒

Definition	The *AB<->TR Conversion* command converts absorbance spectra to transmittance spectra and vice versa. The conversion direction is automatically set by OPUS, depending on the data block stored in the spectrum file.
Principle	Load a spectrum file and select the *AB<->TR Conversion* command. The conversion is immediately performed.

The spectrum displayed by a dotted line (figure 112) has been generated by an AB → TR conversion.
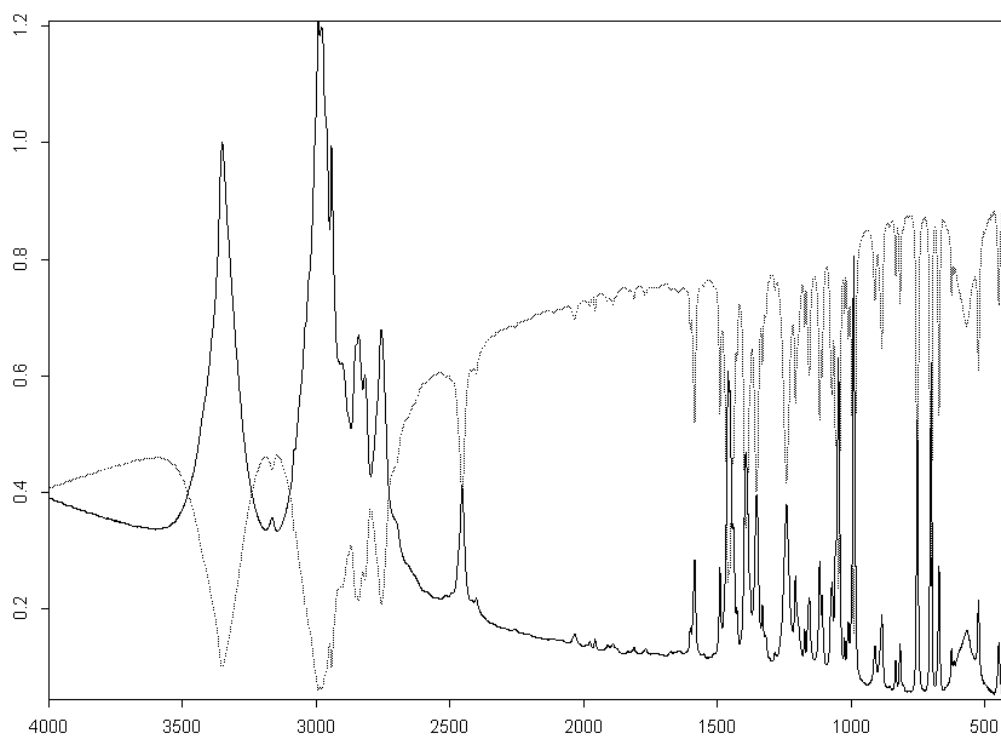
Figure 112: Absorbance spectrum converted into a transmittance spectrum

The equation required for an TR → AB conversion is:

$$AB = -\log(TR)$$

Transmittance values less than 10^{-5} are set to 5 absorbance units.

The equation required for an AB → TR conversion is:

$$TR = 10^{-AB}$$

3.6.4   Spectrum Calculator ▦

Definition	The *Spectrum Calculator* is used to calculate spectra and numerical results. You can also enter algebraic terms.
Principle	The spectrum calculator cannot be compared with a normal pocket calculator. If you enter 100√ into the pocket calculator, you expect the result to be 10. The spectrum calculator, however, operates with algebraic formulae. Therefore, you would need to enter sqrt(100).

Basic features

- To enter figures, signs and functions either use the numerical keypad of your keyboard or click on the spectrum calculator keys. In the latter case inputs will always be added to the entry field (H in figure 113). Delete inputs by using the ⟨-- button.
- If the calculation results in a spectrum, the original spectrum file will be overwritten by the new result spectrum. This also applies to data blocks.
- If two spectra are divided, a transmittance spectrum is generated in the numerator of these two spectra. The transmittance spectrum may overwrite the original spectrum.

To calculate spectra...

...select the *Spectrum Calculator* command to open the following dialog:
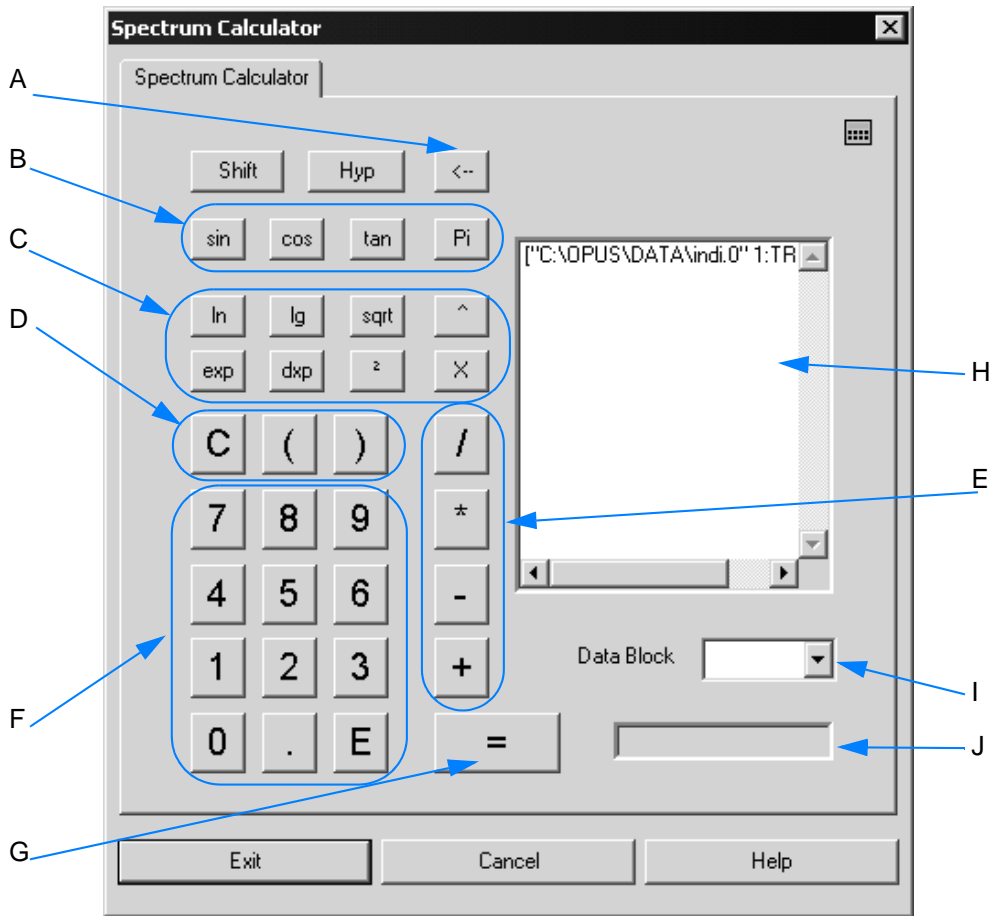
Figure 113: Spectrum calculator

A Use the [<--] button to delete your input.

B These buttons provide trigonometric functions. Additional functions
are available if you use the *Shift* and *Hyp* button:

sin	Sine
asin	Inverse of sine (arcus sine)
sinh	Hyperbolic sine
cos	Cosine
acos	Inverse of cosine (arcus cosine)
cosh	Hyperbolic cosine
tan	Tangent
atan	Inverse of tangent (arcus tangent)

tanh	Hyperbolic tangent
Pi	Trigonometric number π

C The following mathematical functions are available.

ln	Natural logarithm
lg	Logarithm to the base 10
sqrt	Square root
^	Exponent (general)
exp	Exponential function
dxp	Takes the following entry to the base of 10, e.g. 10^x
2	Exponent^2, e.g. $3^2=9$
X	Wavenumber value

D *C* clears the display in (H) and (I). You can use the brackets to form mathematical groups that will be calculated first.

E The four basic arithmetic operations can be used.

F Numerical buttons which consist of the figures 0 - 9, the decimal point and exponential function *E* (e.g. *4.321E3 = 4321*).

G This button starts the calculation. The result will be displayed in the entry field (H).

H The loaded spectrum file to be calculated is available in this entry field. You can also enter algebraic terms and numerical values into this entry field.

I Select the result data block from the drop-down list.

J The display field shows the calculation results, or indicates ERROR in case of an incorrect entry.

Miscellaneous

In some cases it may be necessary to calculate frequency-dependent terms. This can be done using the ⊠ function, which represents the frequency values of the spectral data points. The term

$$\sin(x/100) + [4:TR] - [4:TR]$$

uses the group ([4:TR] – [4:TR]) to generate a spectrum with 0 intensity.

The *x* function causes the frequency limits and data point (frequency) spacing to be applied. The result will be a sine wave.

If you calculated sin (*x*/100) + [4:TR], the spectrum intensity values would be added to the sine wave.

3.6.5   Cut

Definition	The *Cut* command minimizes the frequency range of a data file.
Principle	Load a spectrum file and select the *Cut* command. A dialog opens which automatically contains the name of the spectrum file in the *File(s) to cut* selection field.
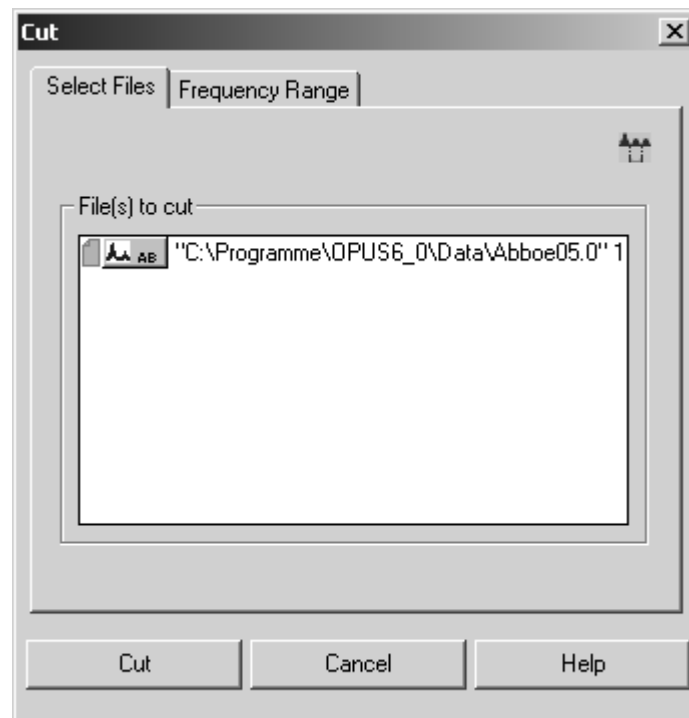
Figure 114: Cut - Select Files tab

1   Click on the *Frequency Range* tab.
2   Define a particular frequency range, see also chapter 1.14.
3   To start the manipulation click on the *Cut* button.

Figure 115 shows a frequency range (thicker curve line) generated by using the *Cut* command.
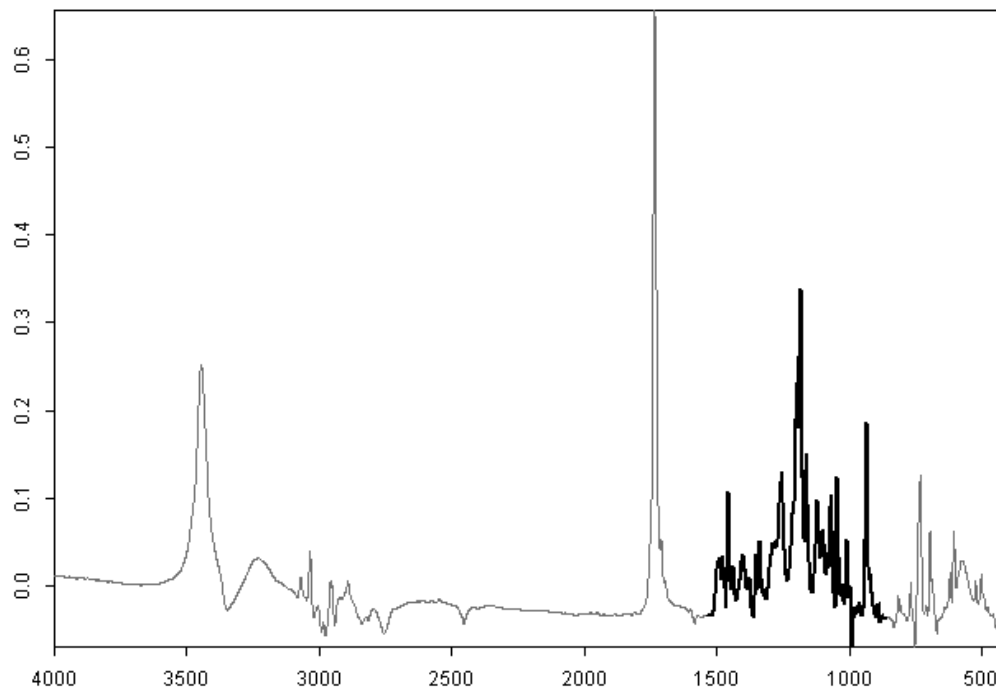
Figure 115: Original spectrum (thin line) and cut-out range (thick line)

You can also use the *Cut* command to invert the frequency limits of spectra.

1   Select upper and lower limits which are beyond the spectral range and define them as new frequency limits in reverse order.

2   Right click on the spectrum and select *Properties* from the pop-up menu.

3   Invert the axes settings using the *Axes* tab. This change may not immediately appear in the spectrum window.

3.6.6   Straight Line Generation

Definition	The *Straight Line Generation* command allows to eliminate fringe effects in the interferogram or artifacts detected in a spectrum.
Principle	Load a spectrum file and select the *Straight Line Generation* command. A dialog opens which automatically contains the name of the spectrum file in the *File(s) for straight line generation* selection field.
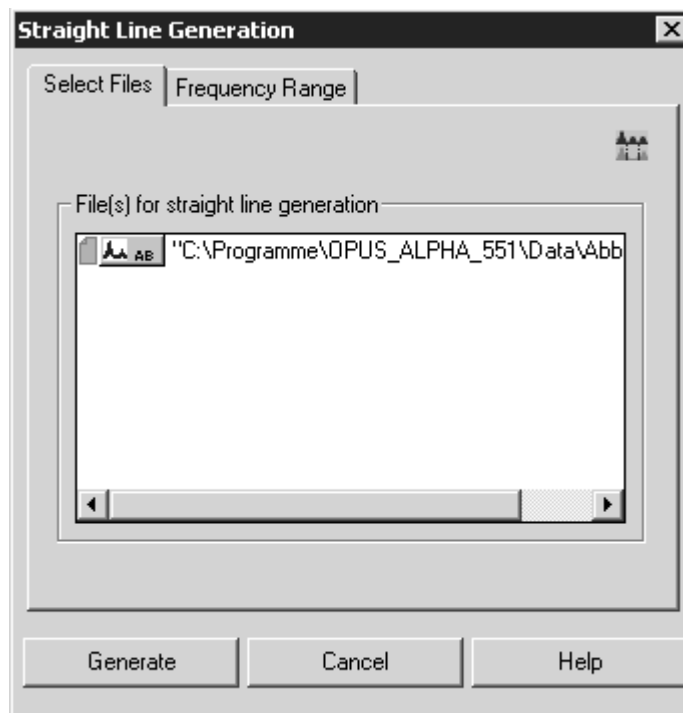
Figure 116: Straight Line Generation - Select Files

1   Click on the *Frequency Range* tab.
2   Define a particular frequency range, see also chapter 1.14.
3   To start the manipulation click on the *Generate* button.

Figure 117 shows a straight line generated between 2,550 and 2,360cm^{-1}, which replaces the original peak (dotted line).
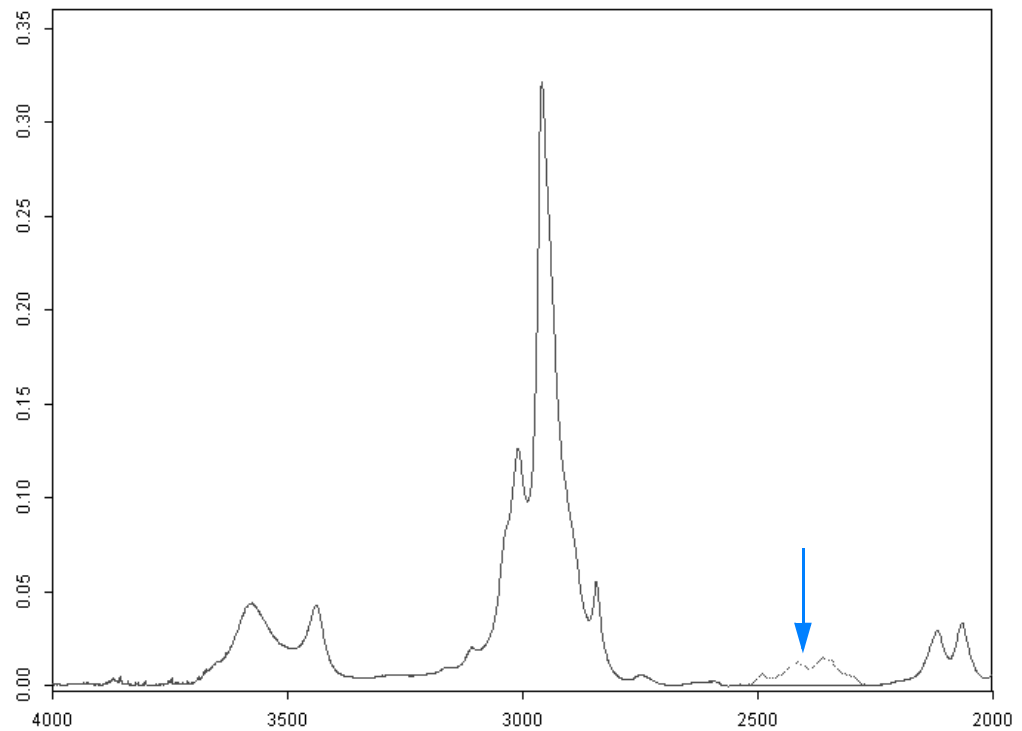
Figure 117: Spectrum before and after generating a straight line

3.6.7   Normalization

Definition	The *Normalization* allows to normalize spectra and perform off-set corrections on spectra.
Principle	Load a spectrum file and select the *Normalization* command. A dialog opens which automatically contains the name of the spectrum file in the *File(s) to normalize* selection field.
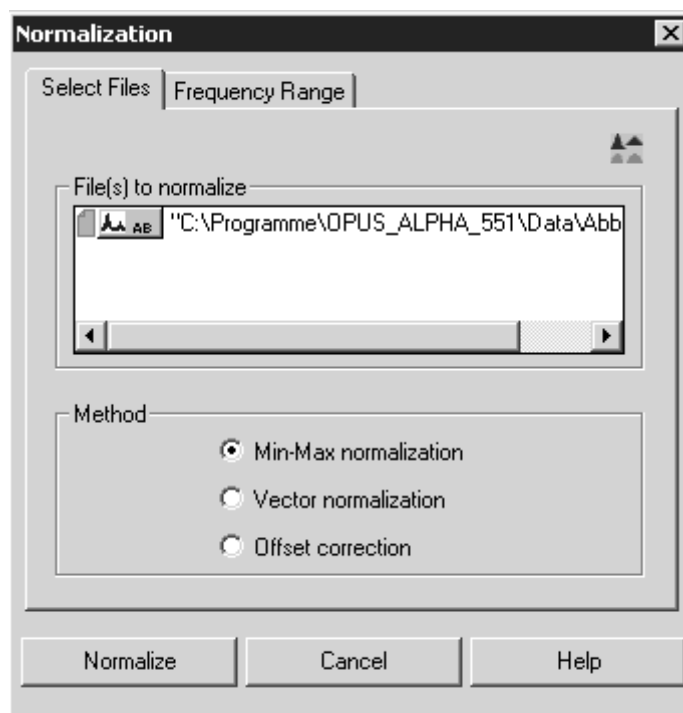
Figure 118: Normalization - Select Files tab

1   Select the appropriate normalization method.

2   Click on the *Normalize* button to start normalization.

Normalization methods

- **Min/Max normalization**

  This method scales spectrum intensities to the effect that the minimum absorbance unit will be 0 and the maximum 2. In case of transmittance spectra the normalization is between 0 and 1.

- **Vector normalization**

  This method calculates the average y-value of the spectrum. The average value is subtracted from the spectrum decreasing the mid-spectrum to y = 0. The sum of the squares of all y-values is calculated and the spectrum is divided by the square root of this sum.

  The vector norm of the result spectrum is 1: $\sum_{i=1}^{NPT} (x_i)^2 = 1$

  with x_i being the spectral intensity of data point *i*.

- **Offset correction**

  This method shifts spectrum intensities to the effect that the minimum absorbance unit will be 0.

3.6.8   Smooth ᴟᴟ᷈ ▾

Definition	The *Smooth* command allows to smooth spectra. As experimental spectra are superimposed more or less by noise interferences it may be required to smooth single spectra.
Principle	The smoothing method is based on the Savitzky Golay algorithm. Possible values for smoothing points are between 5 and 25.

Smoothing...

- ...produces more meaningful spectra.
- ...improves S/N ratio.
- ...can produce over-smooth effects when improperly applied, i.e. single spectra may disappear.
- ...decreases resolution.
- ...reduces spectral noise but also distorts signal intensities.

To smooth a spectrum...

1   ...load a spectrum file and select the *Smooth* command to open the following dialog:
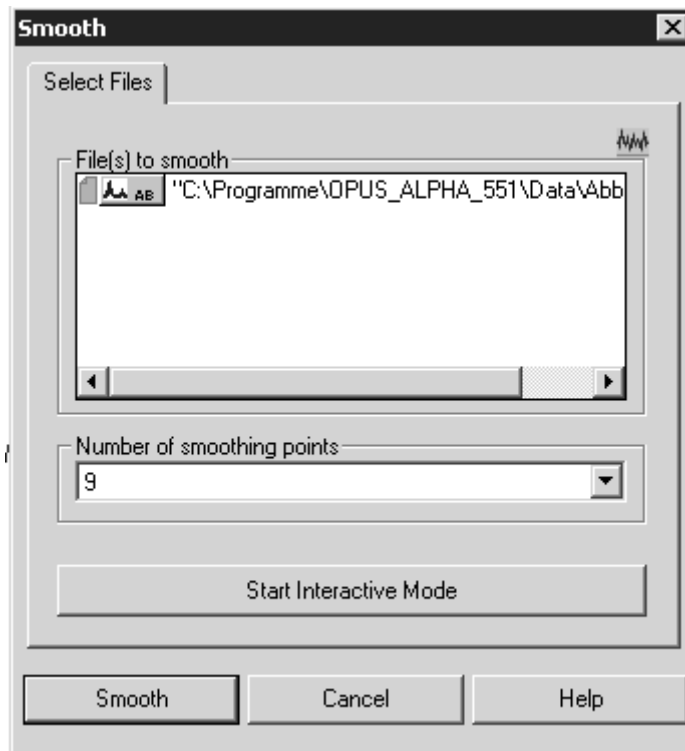
Figure 119: Smooth – Select Files tab

2   Define the number of smoothing points and click on the *Smooth* button to start the command.

Interactive Smoothing

To start interactive smoothing click on the *Start Interactive Mode* button (figure 119). The following dialog opens:
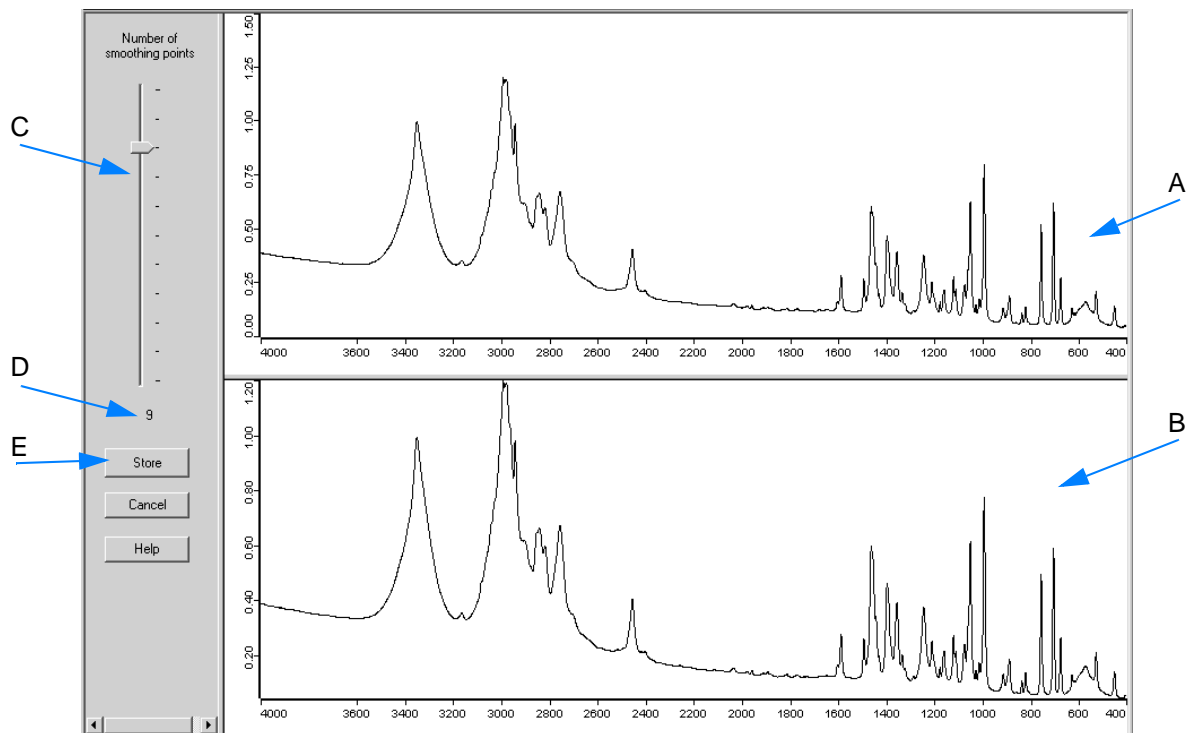
Figure 120: Interactive smoothing

A Original spectrum

B Smoothed spectrum

C Use the slider to set the smoothing points interactively.

D The currently used number of smoothing points is shown below the slider.

E If you click on the *Store* button, the loaded original spectrum file will be changed and the view will close.

Figure 121 directly compares the original spectrum with the smoothed one. The original spectrum band shows more pronounced peaks.
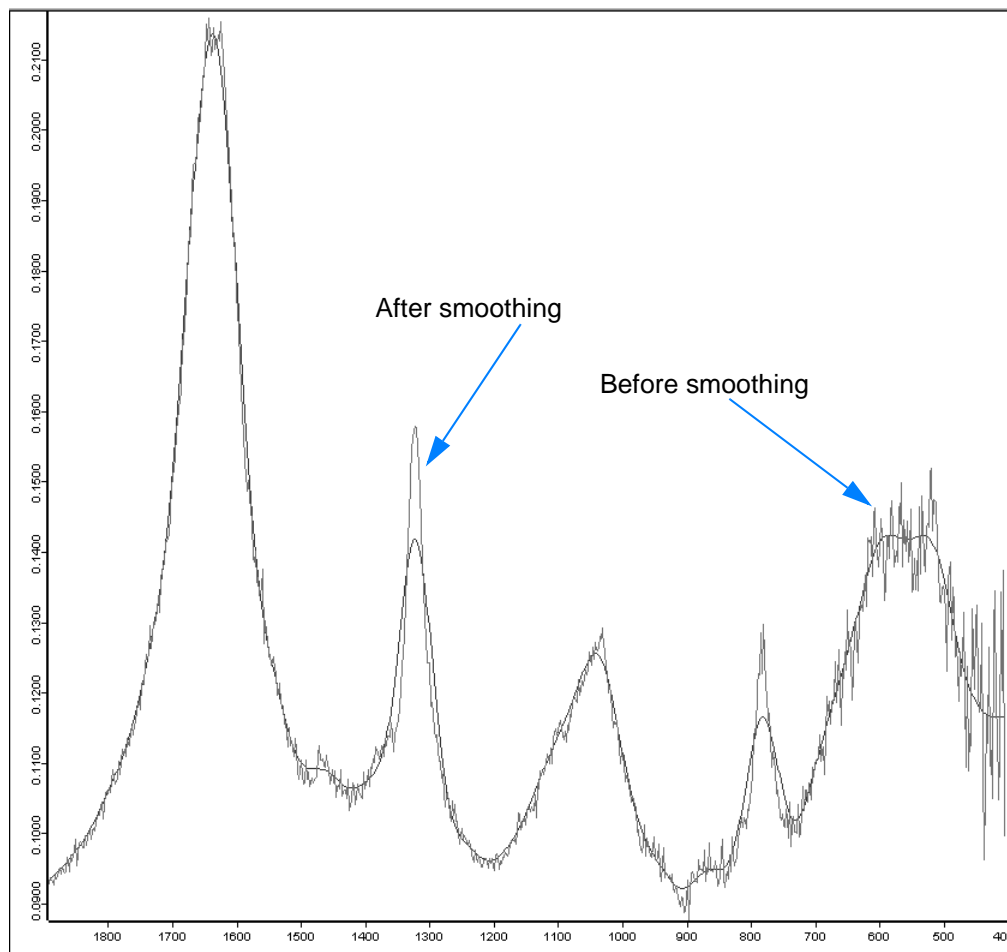
Figure 121: Smoothing effects on a spectrum

3.6.9   Derivative

Definition	The *Derivative* command reduces the background of a signal. This can produce an improved S/N (signal-to-noise ratio).
Principle	The first to fifth derivative of a spectrum is calculated, using the Savitzky-Golay algorithm. This algorithm allows a simultaneous smoothing of the spectrum. The smoothing effect reduces the noise substantially generated by derivation.

To perform a derivative...

1   ...load a spectrum file and select the *Derivative* command to open the following dialog:
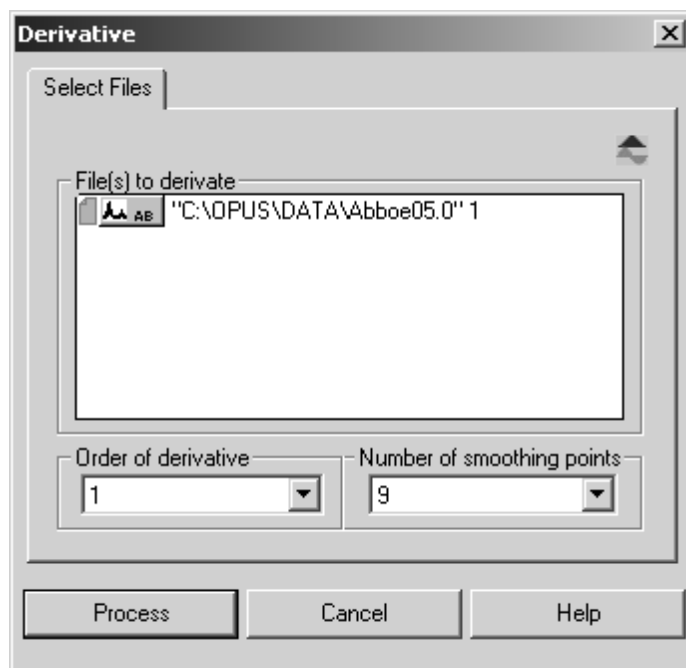
Figure 122: Derivative - Select Files tab

2   Define the number of smoothing points and the derivative order.
Note: The minimum number of smoothing points depends on the derivative order. The higher the derivative order, the more smoothing points need to be set. You can set a maximum of 25 points.

3   Click on the *Process* button to start the derivative.

The derivative result is displayed as...

...a data block indicating the actual derivative order of the original spectrum. If a spectrum of 1st order is subject to a 1st order derivation again, the result will be a 2nd order spectrum. The kind of derivative order is displayed in the data block of the resulting spectrum.

3rd and higher order derivations are symbolized as *n* derivation. The derivative order is stored in the parameters of the derivation data block. Right click on the spectrum file in the browser and select *Show parameters* from the pop-up menu.

3.6.10 Convert Spectra ⊞

Definition	The *Convert Spectra* command includes several conversion methods which mainly involve the display of the spectra.
Principle	When selecting spectrum files for conversion certain restrictions may apply. If you try to select a spectrum which does not comply with the conversion method selected, a warning symbol will be displayed.

1   Load the spectrum file and select the *Convert Spectra* command.

2   A dialog opens which automatically shows the name of the spectrum file in the *File(s) to convert* selection field.
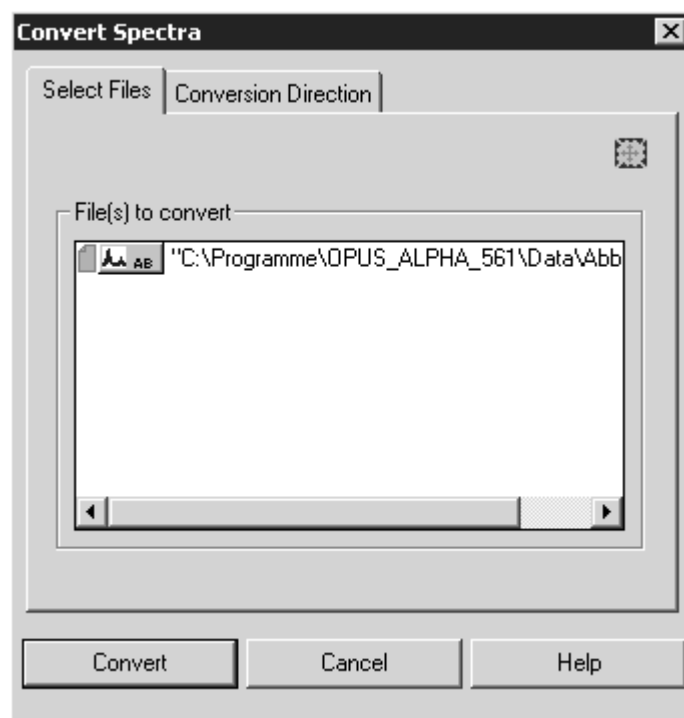
Figure 123: Convert Spectra

3   Define the diversion method on the *Diversion Direction* tab.
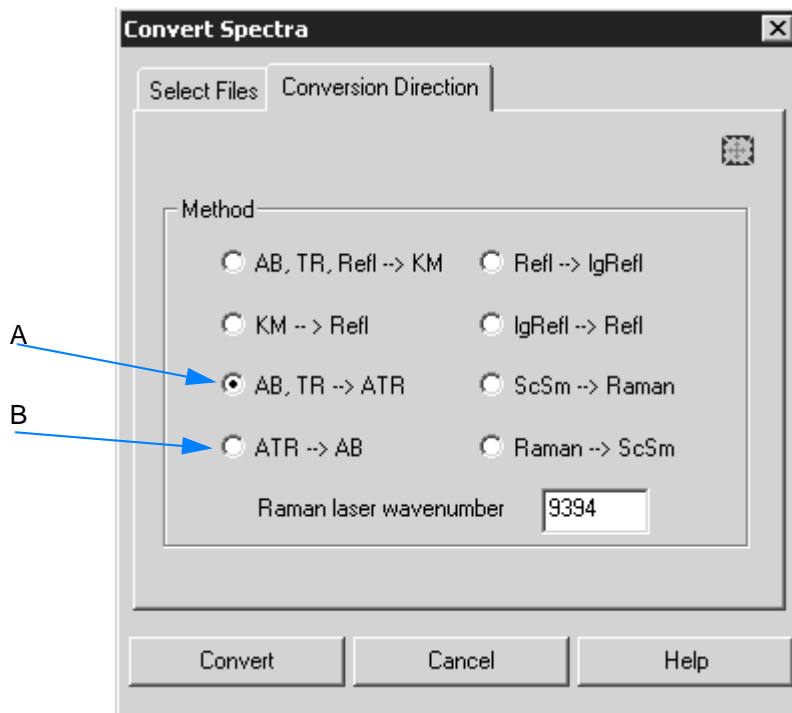
Figure 124: Convert Spectra - Conversion direction

> 4   Start the conversion by clicking on the *Convert* button.

Conversion Method

When working with the ALPHA spectrometer only the conversion method A and B in figure 124 are suited for spectra conversion.

- A: Converting to ATR spectra (ATR correction is performed)
- B: Converting to absorbance spectra (ATR correction is undone)

When **performing ATR correction** the following conversion formula is applied:

$$ATR = AB \cdot \frac{X}{1000}$$

with *X* being the wavenumber. Transmittance spectra are first converted to absorbance spectra. As in case of ATR (Attenuated Total Reflection) measurements the penetration depth is inversely proportional to the wavenumber (frequency), the spectra are normalized to a constant penetration depth.

When **converting ATR spectra to absorbance spectra** the following conversion formula is applied:

$$ATR = AB \cdot \frac{X}{1000}$$

3.6.11 Atmospheric Compensation

Definition	The *Atmospheric Compensation* command allows to eliminate disturbing H_2O and/or CO_2 bands in ratio spectra. These bands arise due to different H_2O/CO_2 vapor concentrations in the beam path if you measure reference or sample spectra, respectively.
Principle	To perform atmospheric compensation a single-channel reference spectrum and single-channel sample spectrum are analyzed and transformed into a ratio spectrum without any (or hardly any) H_2O and/or CO_2 bands. Load a spectrum file and select the *Atmospheric Compensation* command.

The *Atmospheric Compensation* command uses physical models to estimate the amount of atmospheric gases in the single-channel spectra and therefore compensates disturbing H_2O and/or CO_2 bands.

Note: As atmospheric compensation manipulates the original data it has to be used with due care.

What kind of spectrum is required?

Two single-channel spectra:

- single-channel sample spectrum
- single-channel reference spectrum

What kind of spectrum features have to be considered?

- **Wavenumber ranges:**
  - for H_2O compensation: from 3600 to 4000cm^{-1}
  - for CO_2 compensation: from 2300 to 2400cm^{-1}

- Sample absorption within these wavenumber ranges will result in poorer quality with regard to compensation.
- The sample and reference spectrum have to be acquired using the same spectrometer resolution. Different zero-filling factors are possible.
- The spectrum should not end at a wavenumber which shows strong absorption of atmospheric gases. In case of a H_2O compensation (see figure 128), the lower wavenumber limit **must not** be around 1700cm^{-1}.
- For compensation in aqueous solutions the spectrum has to include wavenumber ranges of 2300-2400cm^{-1} and 1800-1900cm^{-1} for both CO_2 and H_2O. These wavenumber ranges must be free of sample absorption bands.

What about the spectrum file?

Make sure that the two single-channel spectra which belong together are uniquely defined as data block in the spectrum file.

Example:
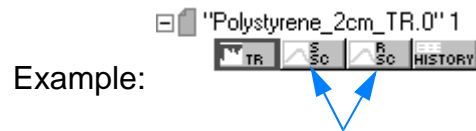
If the spectrum file **additionally** contains a ratio spectrum (AB or TR), it is also possible to perform atmospheric compensation by using this kind of spectrum.

When loading a spectrum file which does not contain the required single-channel spectra, a warning pops up.

Figure 125: Atmospheric Compensation - Warning

When using atmospheric compensation as part of the measurement process....

...there are two possibilities:

- **Use the wizard**

    Click on the *Atmospheric Compensation* button on the *Manipulate* level.
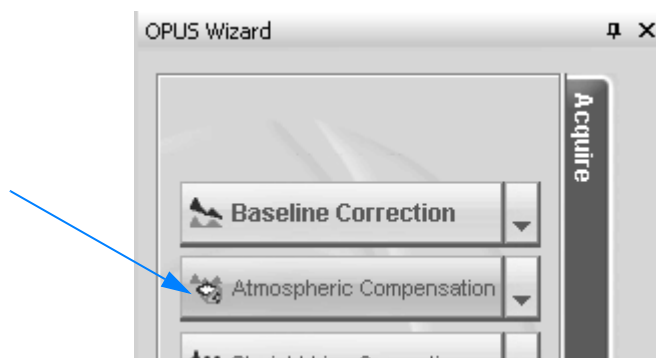
Figure 126: Atmospheric compensation in the wizard

The manipulation command is immediately performed.

- **Define atmospheric compensation in the measurement parameter**

  Select the *Setup Measurement Parameters* command in the *Measure* menu. Activate the check box *Atmospheric compensation* on the *Setup Measurement Parameters* dialog. In this case an atmospheric compensation will immediately be performed after each measurement.
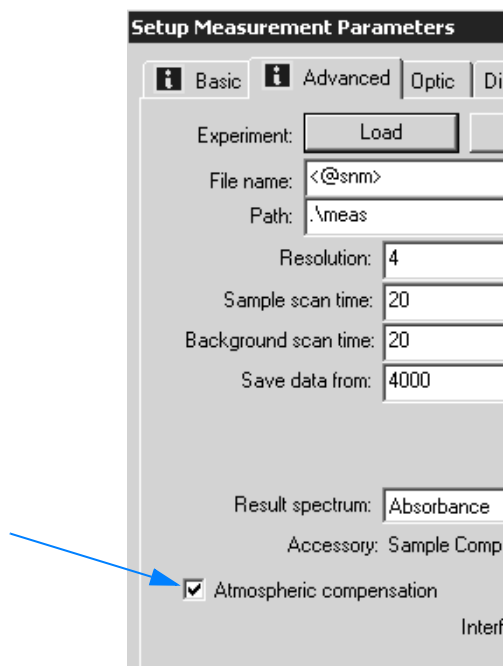
Figure 127: Atmospheric compensation measurement parameter

Figure 128 shows atmospheric compensation effects.
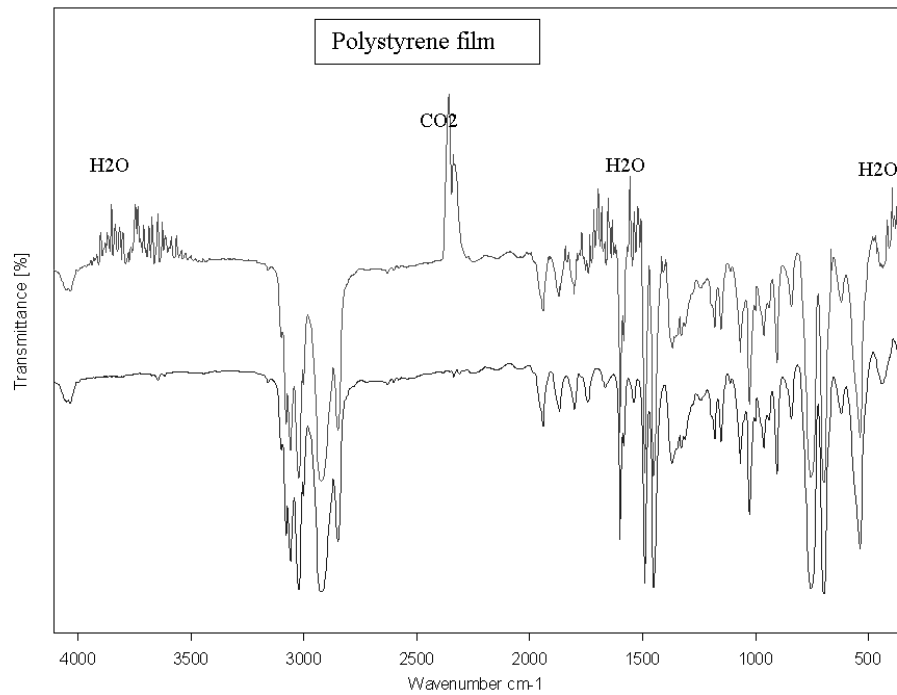
Figure 128: Atmospheric compensation effects

The upper curve is the transmission spectrum of a polystyrene film. H_2O and CO_2 bands can be clearly seen in several wavenumber ranges. The lower curve is the result of atmospheric compensation. Disturbing absorption lines of H_2O and CO_2 have nearly been eliminated.

3.7   Evaluate Menu

The commands included in the *Evaluate* menu primarily intend to calculate results from existing spectra. This could be a quantitative data analysis, peak identification or a library search. These calculations do not alter the spectrum files.
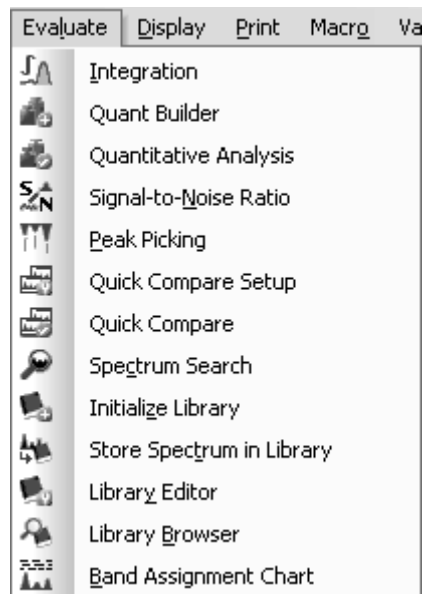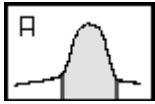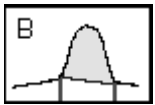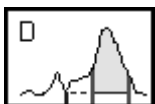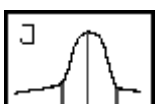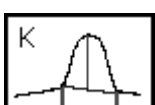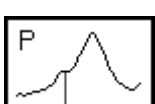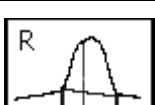
Figure 129: Evaluate menu

3.7.1   Integration

Definition	The *Integration* command allows the integration of peaks as well as the calculation of peak heights.
Principle	An integration method is required first to be able to perform an integration. This method includes the integration mode and the frequency ranges to be considered to integrate spectra. Integration methods have the extension *.INT* and can be stored separately in the *C: Program\OPUS\Method* default path.

Integration modes

The following integration modes are available:

A	The integration will be performed between the band, abscissa and the frequency limits defined.
B	A straight line is drawn between the peaks of the two frequency limits defined. The area above this line will be integrated.
D	The baseline is horizontal and determined by the baseline point defined.
J	Highest absolute peak intensity
K	Peak intensity relative to the local baseline
P	Peak intensity at the specified frequency
R	Peak intensity at a given frequency

One particular spectrum can be integrated several times by using different integration methods.

Before you can start an integration...

...you first have to create an integration method. An integration method specifies the frequencies for one or more areas which are to be integrated.

3.7.1.1 Creating an integration method

Load a spectrum file and select the *Integration* command to open the following dialog:
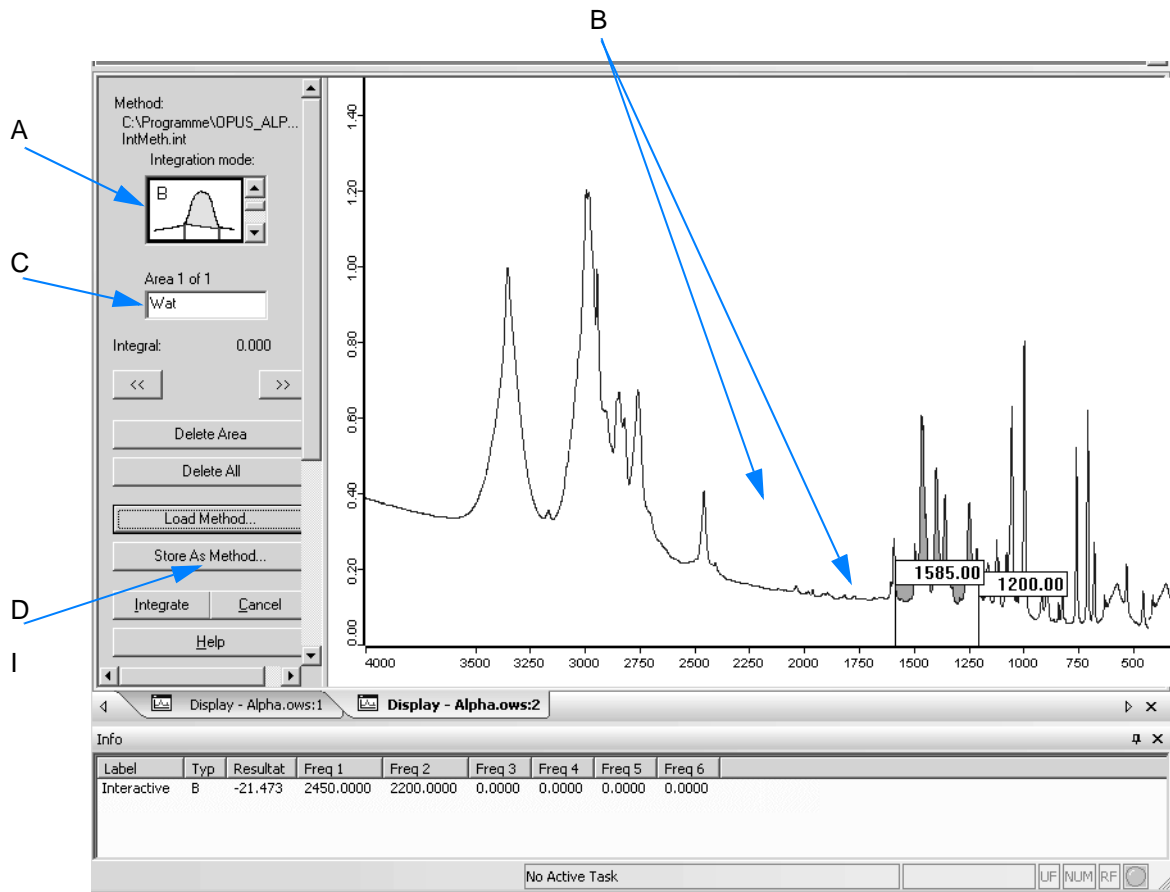
Figure 130: Integration - Interactive method setup

> 1   Select an appropriate integration mode (A) available in OPUS.
>
> 2   Define an integration area (B). Left click into the spectrum and draw a line between two limits. The limits of the integration area are displayed by the exact wavenumber.
>
>   Activated integration areas are displayed in red (I in figure 131), non-activated areas are displayed in light red (II).
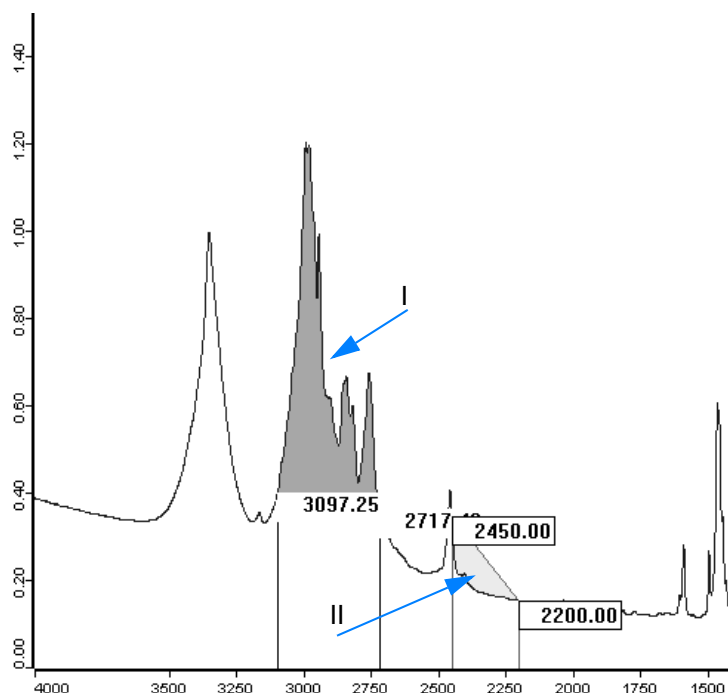
Figure 131: Activated and non-activated integration areas

3　Each integration area can be defined by a certain name. Enter this name into the entry field (C in figure 130). To change between different integration areas use either the forward (>>) or backward (<<) arrow buttons.

4　Store the current settings made as integration method by clicking on the *Store As Method* button (D).

5　Another dialog opens. Specify the method file name and define the path.

To change the limit of an integration area...

- ...you first have to select the area.
- If you position the cursor on the area edge, the cursor will change into ⟷. Now, you can move the limit to the position desired.
- It is also possible to left click somewhere below the spectrum, draw a line and release the mouse button. The area selected will then be highlighted. To edit the wavenumber displayed, click into the respective entry field.

3.7.1.2 Performing an integration

1   Load a spectrum file by means of the wizard. Click on the *Load File* button on the *Acquire* level.

2   Go to the *Evaluate* level. Click on the *Integration* button or select the command from the drop-down list. In the latter case click on the *Go* button.

3   The integration is immediately performed, **provided you have defined an integration method before. If no integration method is available, a warning pops up.**

4   The integration area is displayed in the spectrum window.
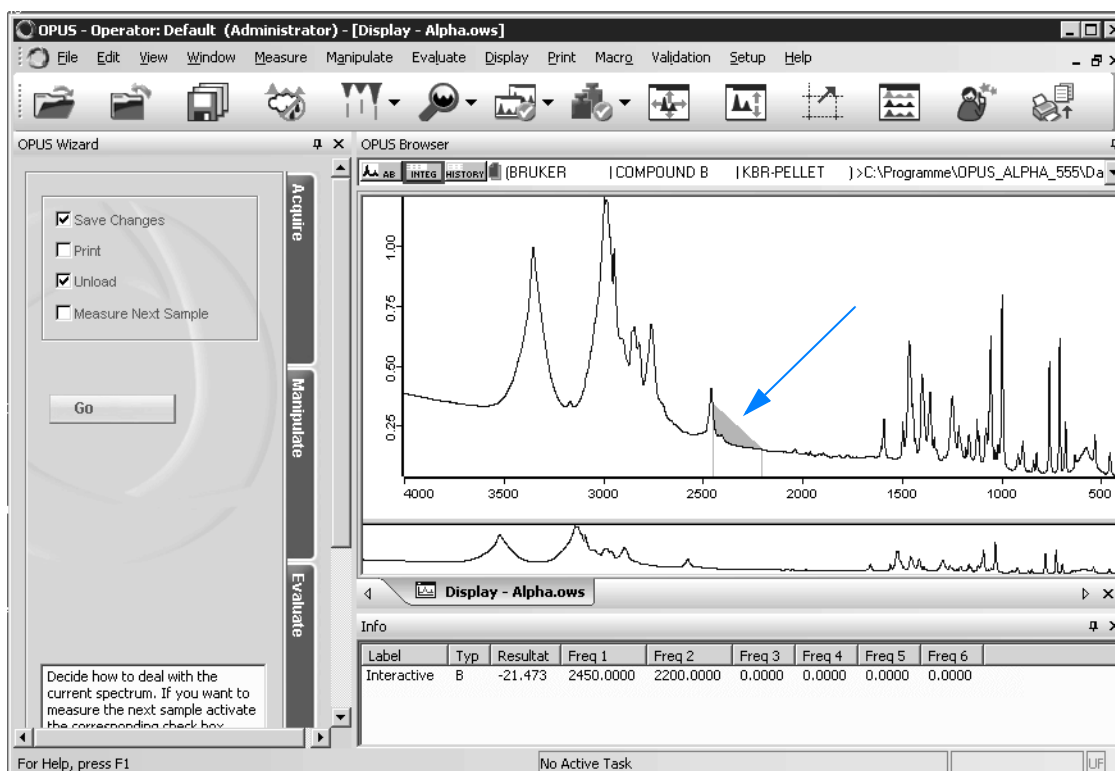
Figure 132: Integration area displayed in the spectrum window

The integration result is stored...

...in the integration data block ([INTEG]).

To display integration results in a report window...

...right click on the [INTEG] data block in the browser and select the *Show Report* option from the pop-up menu. The report window opens and contains the name of the integration mode selected, the name of the area as well as the frequency limits.
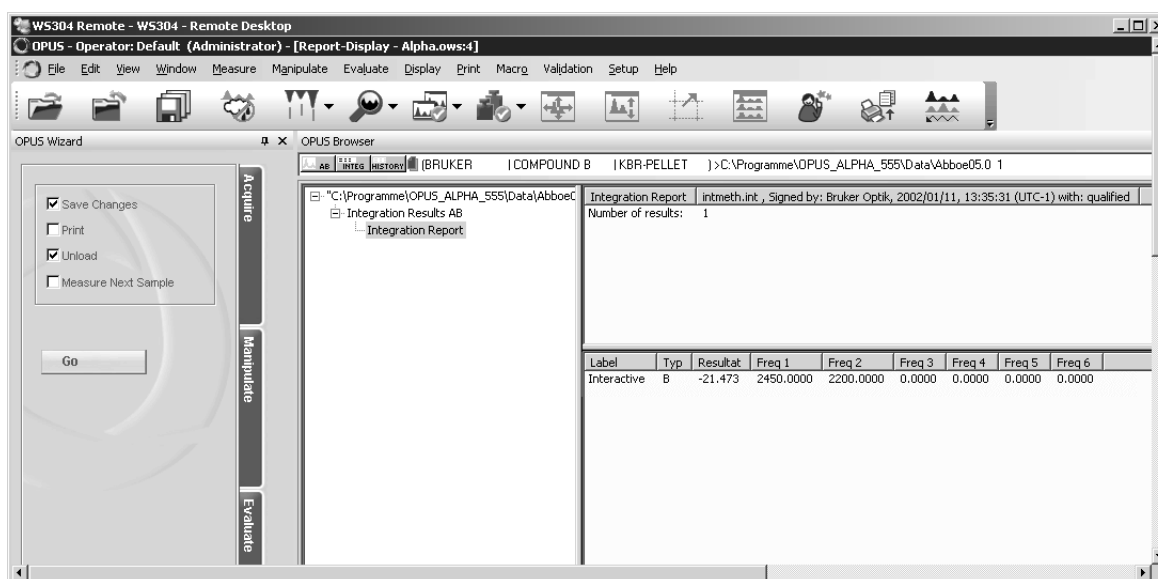
Figure 133: Integration - Report window

To print the integration areas and modes together with the spectrum...

1   ...click on the *Print Spectra* command.

2   Click on the *Change Layout* button and select a layout which contains a spectral frame, e.g. *spectrum_Integ.PLE,* using the *C:Program\OPUS* directory.

3   To get a preview of the spectrum and the integration areas click on the *Show preview* button.

4   Click on the *Print* button.

3.7.2   QUANT Builder

Definition	The *QUANT Builder* command allows to setup a QUANT method during sample measurement.
Principle	Perform a sample measurement after the background measurement has been completed. Use the QUANT Builder for each single sample measurement required to add to the QUANT method.

A QUANT method consists of:

• Concentration values of sample component
• Spectra
• Integration area

In case of a QUANT method...

...calibration spectra are required. This so-called set of calibration samples should contain the component to be analyzed in various concentration values. The concentration value of this component in each single sample has to be known.

Note: The set of calibration samples should contain at least 5 samples.

For detailed information on the set of calibration samples refer to chapter 2.4.2.

How to work with QUANT Builder?

1   Measure the first sample by clicking on the *Measurement* button in the wizard. The *Measurement* dialog opens.

2   Start a background measurement **before** the sample measurement. Click on the *Start Background Measurement* button. **Note: In case of a background measurement there is no sample in the sample compartment (transmission) or on the ATR crystal. This kind of measurement is also called reference measurement**. For further details refer to chapter 2.1.2 and 3.5.2.
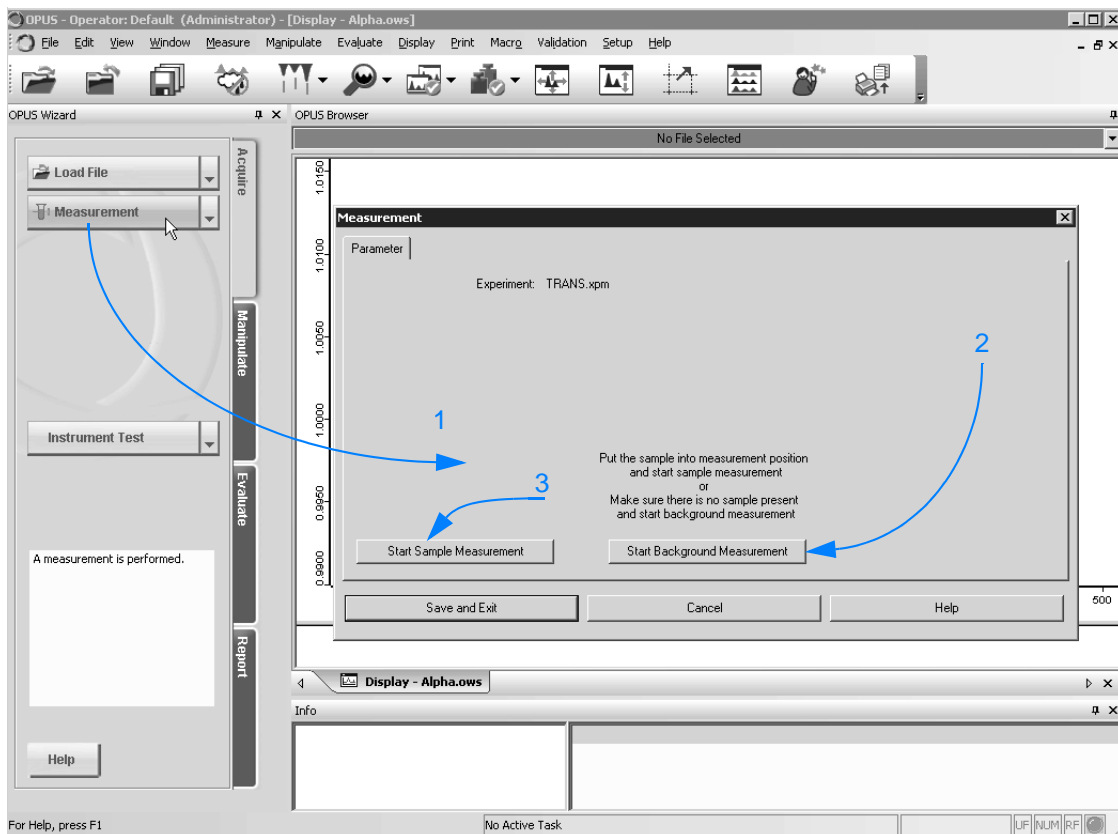
Figure 134: QUANT Builder - Performing measurement

3   Start the sample measurement. Click on the Start *Sample Measurement* button. **Tip: In case of sample measurements it is recommended to have the sample name prompted before each single measurement. Therefore, define this parameter when setting up new measurement experiments.**
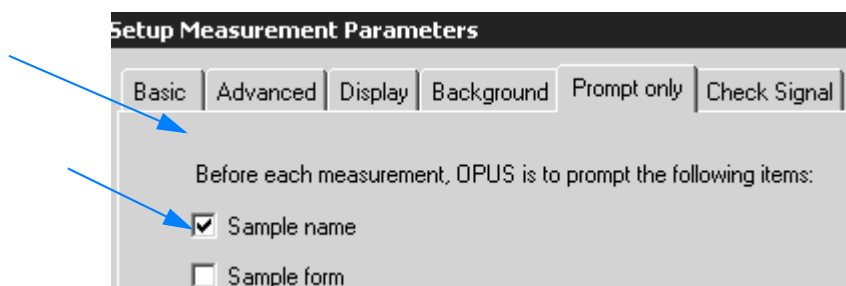
Figure 135: Parameter: Prompt sample name

4   If the sample measurements have been completed, open the QUANT Builder. Click on the appropriate button on the wizard *Evaluate* level or select *QUANT Builder* from the drop-down list. In the latter case click on the *Go* button to open *QUANT Builder*.
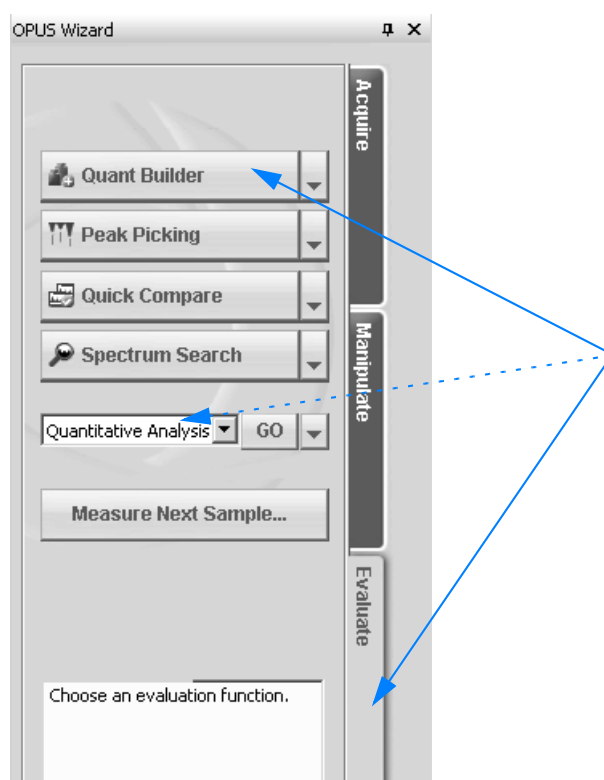
Figure 136: Wizard - QUANT Builder

5   The *QUANT Builder - New* dialog is displayed.
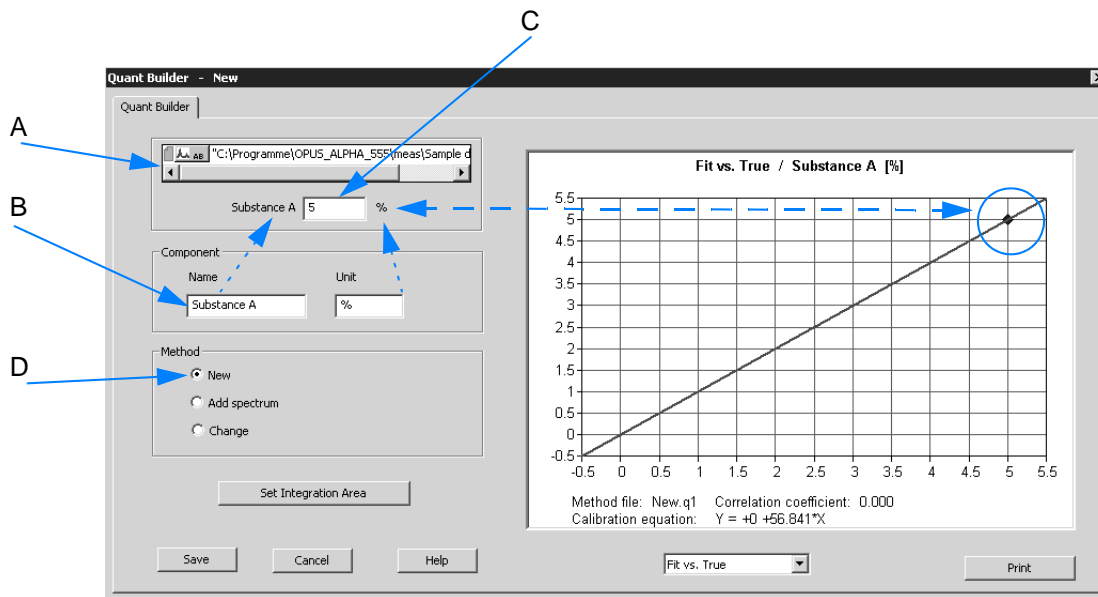
Figure 137: QUANT Builder

6   The selection field (A in figure 137) contains the spectrum file name of the sample measured before.

7   Enter the name (B) of the component to be analyzed as well as the unit (e.g. mg, % etc.). The entries made are displayed above (see broken arrow lines in figure 137).

8   Enter the concentration value of the component. On the basis of this value and the corresponding spectrum a calibration straight line is calculated. The concentration value is displayed on this calibration straight line. **If you have entered a wrong concentration value, write the correct value into the entry field.**

9   When creating a new method, the *New* option button (D) is activated by default.

10 Define one isolated peak for the component, which peak height or integral is to be used for calibration. Click on the *Set Integration Area* button to open the following dialog:
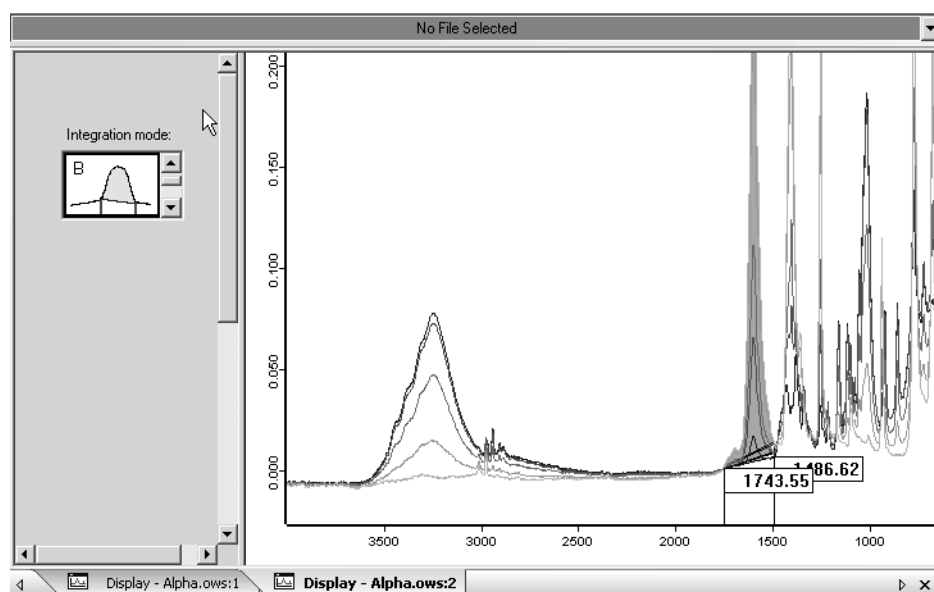
Figure 138: Define integration area

- Select an integration mode. For detailed information on the single integration modes refer to chapter 3.7.1.
- Define the integration area. If you position the cursor on the area edge, the cursor will change into ⟷. Now, you can move the limit to the position desired. **Note: Set the integration area such, that the band of the sample component to be analyzed is within this integration area.**
- Return to *QUANT Builder* by clicking on the *Go to QUANT* button.

Storing QUANT method

1   Click on the *Save* button in *QUANT Builder*.
2   The following dialog opens:
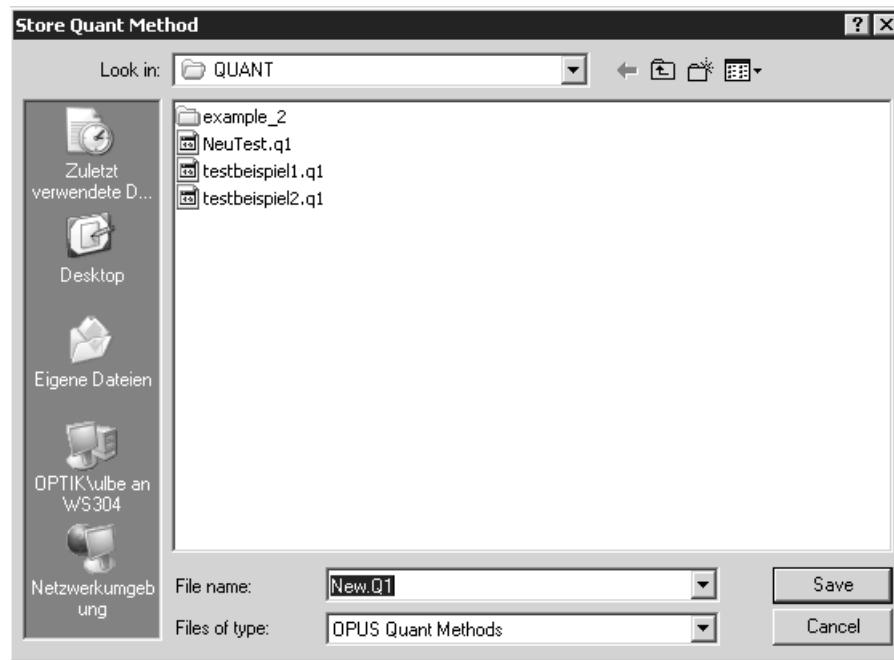
Figure 139: Storing QUANT method

3   Enter the desired method file name and define the path. QUANT methods have the extension *.Q1*.

4   If the settings have been made, click on the *Save* button.

Measuring further samples

Measure all samples required for the set of calibration samples. Repeat the steps described above for each sample by means of *QUANT Builder*.

> **Note: Measuring the second and all subsequent calibration samples does not require to create a new method. It is possible to add the spectrum/spectra to the method currently used.**

The *Add Spectrum* option button is activated in *QUANT Builder*.
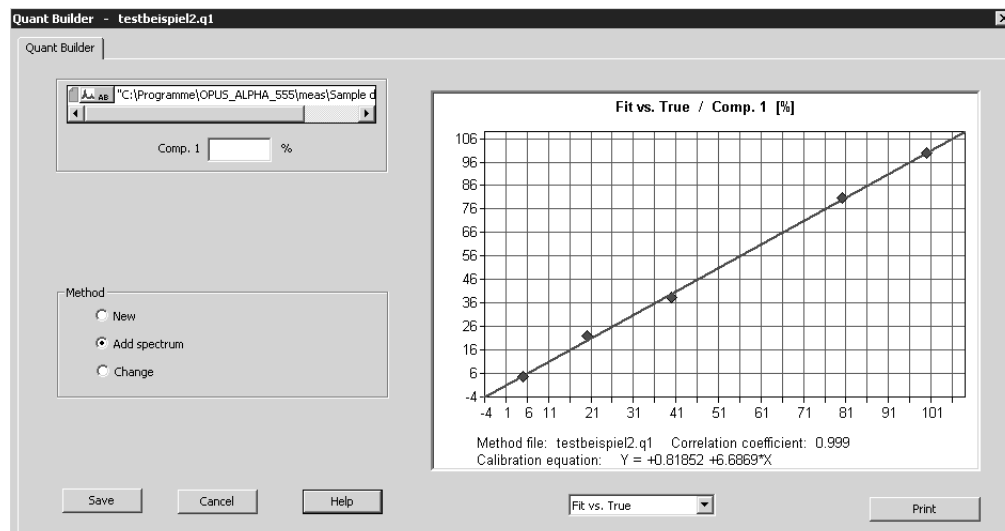
Figure 140: QUANT Builder - Add spectrum

> **Note: Click on the *Save* button to allow the spectrum to be added to the current method. If you click on the *Cancel* button, the current method will not be modified.**

QUANT Builder closes after saving the method. Continue sample measuring by clicking on the *Measure Next Sample* button on the *Evaluate* level in the wizard.
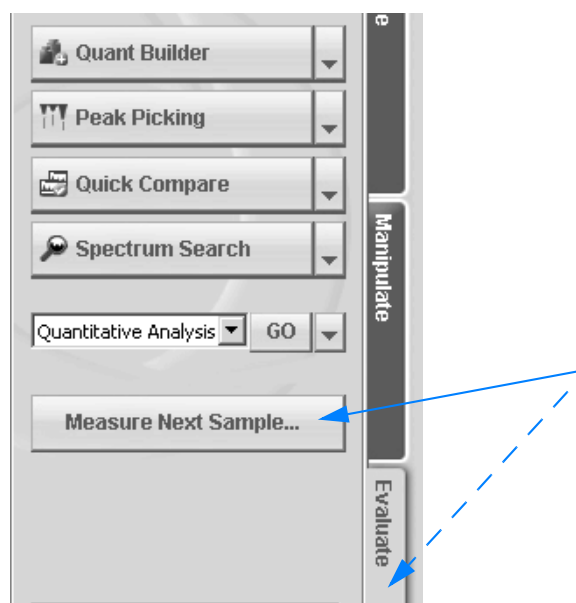
Figure 141: Wizard - Measure next sample

Changing QUANT method

Activate the *Change* option button in *QUANT Builder*. The dialog is displayed as follows:
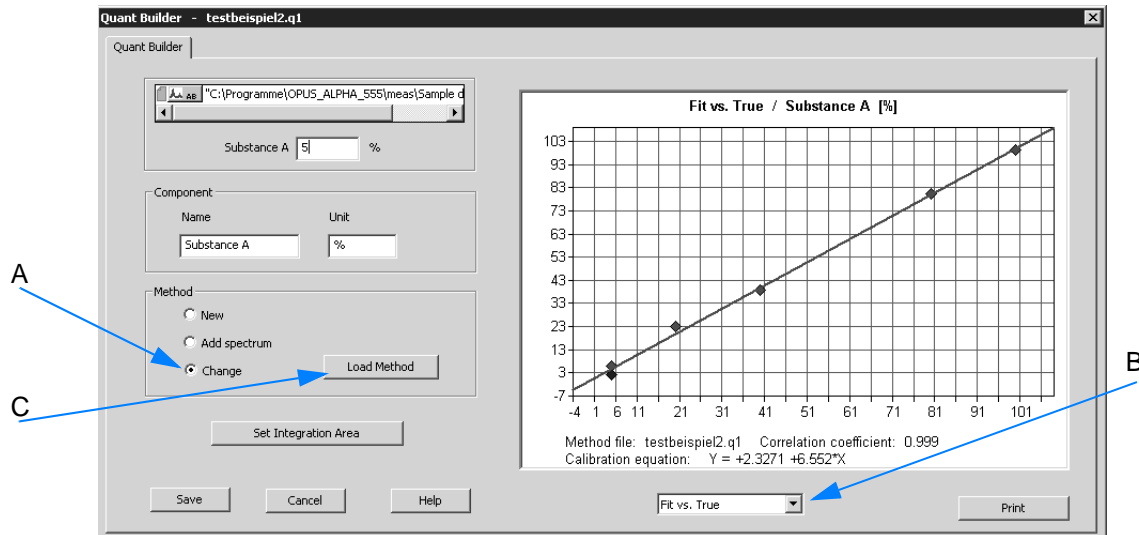
Figure 142: QUANT Builder - Change method

A Activate this option button if the current method is to be changed. The following changes are possible:
- Value of component
- Name of component
- Integration area

B Select a depiction type for the calibration graph. The following types are available:
- **Fit vs True** (adaptation against the known component value
- **Difference vs True** (difference against the known component value)
- **True vs X** (applying known component value against intensity of bands

C Use the *Load Method* button to load an already existing method.

To delete a particular calibration spectrum from the graph double click onto the spectrum.

If all changes have been set, click on the *Save* button.

3.7.3   Quantitative Analysis

Definition	The quantitative analysis allows to determine the concentration value of a specific sample component.
Principle	Load a spectrum file and select the *Quantitative Analysis* command. A dialog opens which automatically shows the name of the spectrum file in the *File(s) for Quantitative Analysis* selection field. **Note: A quantitative analysis can only be performed if you have created a QUANT method first, see chapter 3.7.2.**
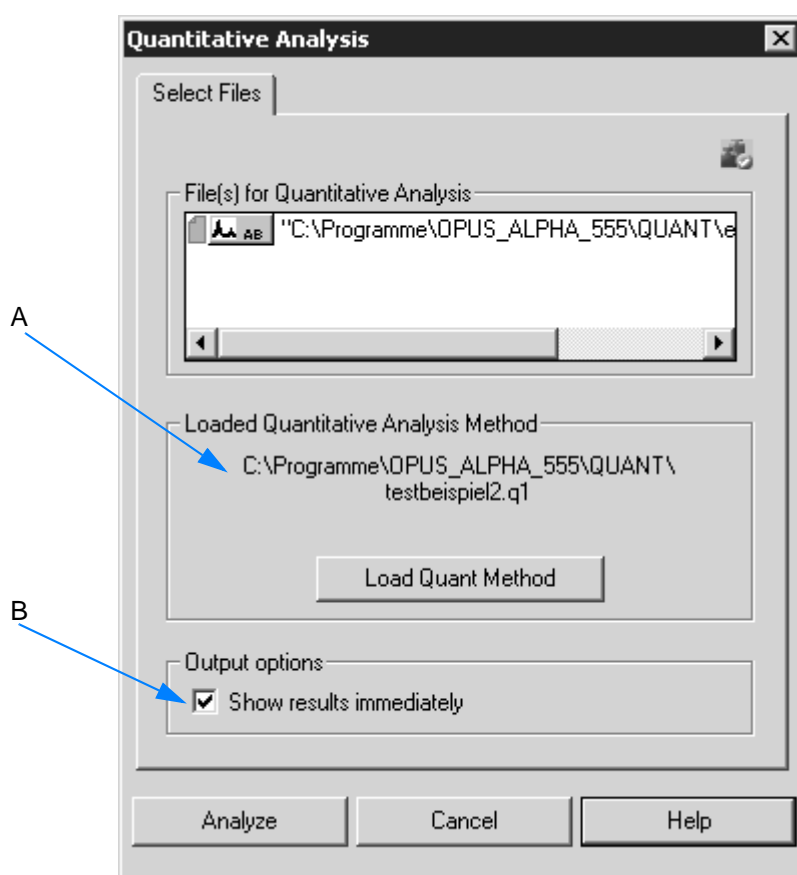
Figure 143: Quantitative Analysis - Select Files

1   Load a QUANT method if no QUANT method is displayed or if you want to use a different method than displayed. Click on the *Load QUANT Method* button and select the respective method from the dialog. **Note: By default, the dialog shows the name of the QUANT method recently used** (A in figure 143).

2   Activate the *Show results immediately* option box (B). The quantitative analysis results are directly displayed after the analysis has been performed.

3   Click on the *Analyze* button to perform the analysis.

The result of a quantitative analysis...

- ...is displayed in a specific view (see also chapter 2.4).

Result of QUANT evaluation:

Component	Prediction	Sigma	Unit	Integr. Result
Comp. 1	4.63	1.51	%	0.57

Figure 144: Result of quantitative analysis

- ...is stored in the QUANT data block ([QUANT]) together with the spectrum analyzed.

To display the quantitative analysis result in a report window...

...right click on the [QUANT] data block in the browser and select the *Show Report* option from the pop-up menu.

The report window opens and contains the name and date of the analysis method, as well as the name of the component which has been analyzed (see also chapter 2.4).
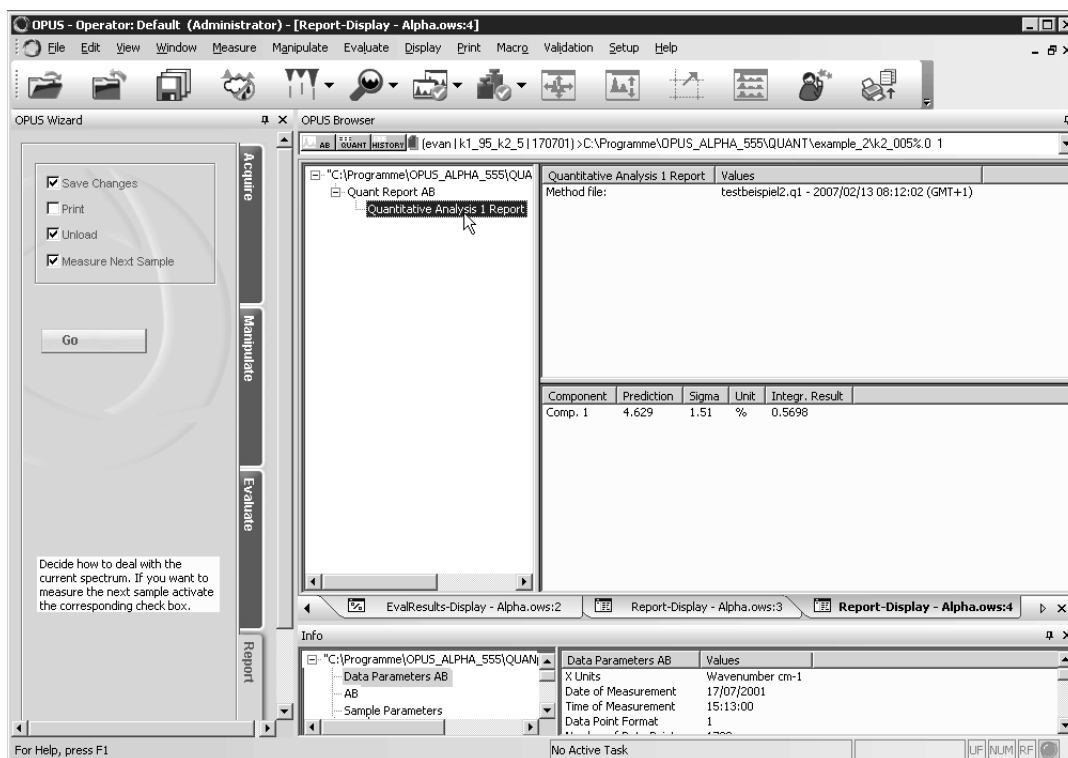
Figure 145: Quantitative Analysis - Report window

3.7.4   Signal-to-Noise Ratio

Definition	This command calculates the signal-to-noise ratio (S/N) of a spectrum within a given frequency range.
Principle	A curve is fitted to the spectrum in the specific frequency range. This curve is either a straight line or (optionally) a quadratic parabola, and defines the (nominal) signal. The (mean) nominal signal is divided by the calculated noise values and yields the S/N. **Note: This command is only reasonable in case of spectra with a baseline close to 0.**

Calculating S/N

1 Load an appropriate spectrum by means of the wizard. Click on the *Load File* button on the *Acquire* level.

2 Go to the *Evaluate* level. Click on the *Signal-to-Noise Ratio* button or select the command from the drop-down list. In the latter case click on the *Go* button to perform the calculation.
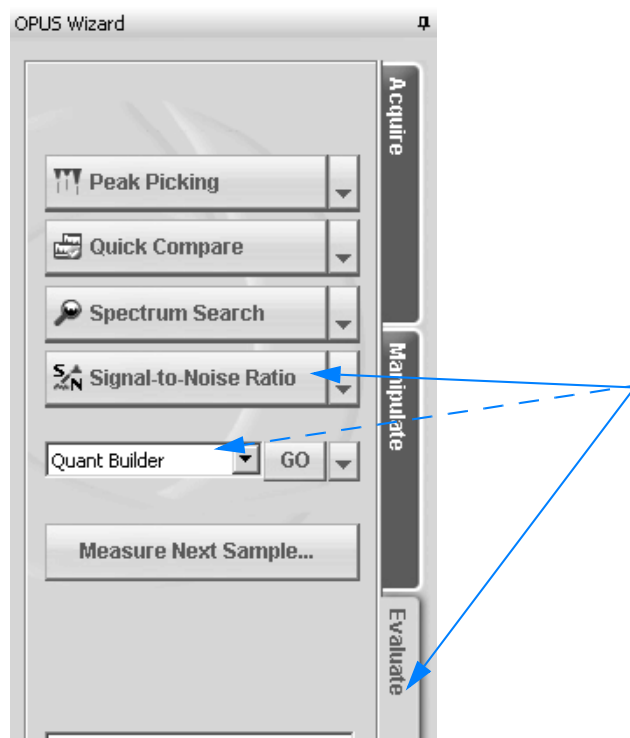
Figure 146: Wizard - Signal-to-Noise Ratio

3 The calculation is immediately performed.

4 A dialog pops up and contains the calculation result. *Minimum* and *Maximum* gives the extrema of the ordinate values of the evaluated range.
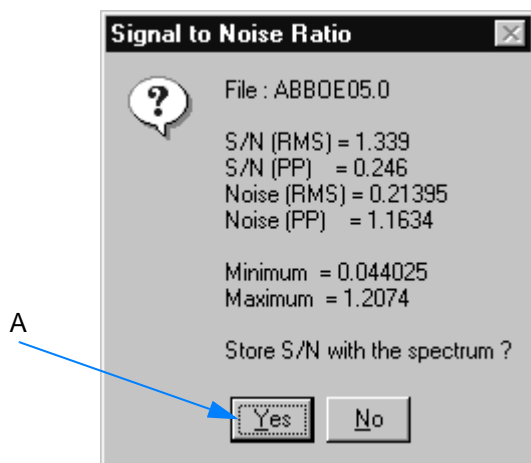
Figure 147: Calculated S/N result

To store the result...

...click on the *Yes* button (A in figure 147). The OPUS spectrum window displays the spectrum with the calculated S/N ratio.

Result displayed in parameters' list

The S/N results are stored together with the spectrum in a parameters' list. This list can be viewed by right clicking on the spectrum file name in the OPUS browser window. Select the *Show Parameters* command from the pop-up menu. The following view is displayed

Figure 148: Report with SN data parameters

Note: The parameters are also displayed in the *Info* view below the spectrum window.

To change calculation settings...

1   ...load the spectrum file and select the *Signal-to-Noise Ratio* command from the *Evaluate* menu.

2   The following dialog opens which automatically shows the name of the spectrum file in the *File(s) to compute signal to noise* selection field:
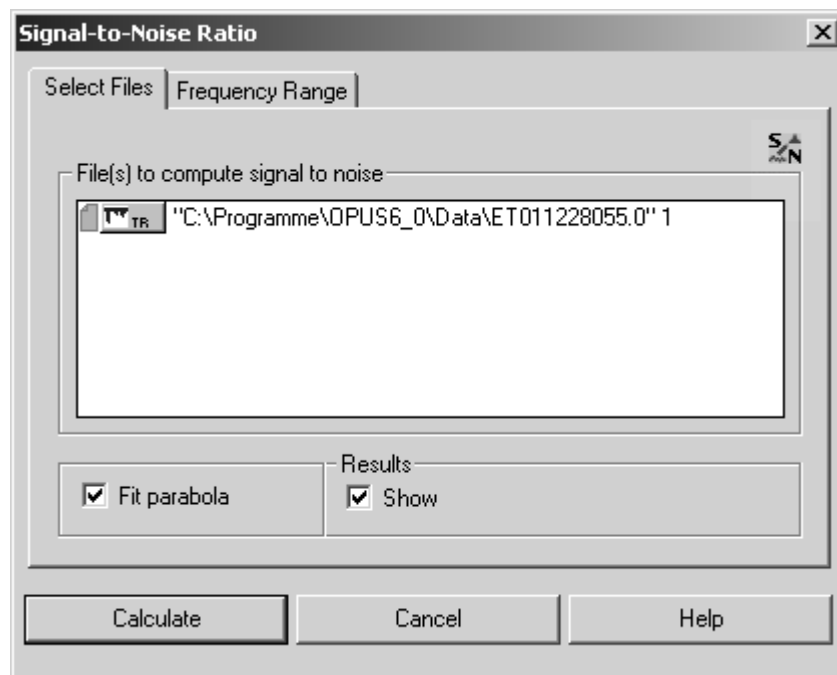
Figure 149: Signal-To-Noise Ratio - Select Files

3   You can activate the *Fit Parabola* check box, otherwise a linear function is automatically fit to the data.

4   If you deactivate the *Show* check box, the results of the calculation will not be displayed.

5   On the *Frequency Range* tab you can select between different pre-defined frequency ranges. Select the frequency range either interactively or use the current file limits. For detailed information on how to define frequency ranges refer to chapter 1.14
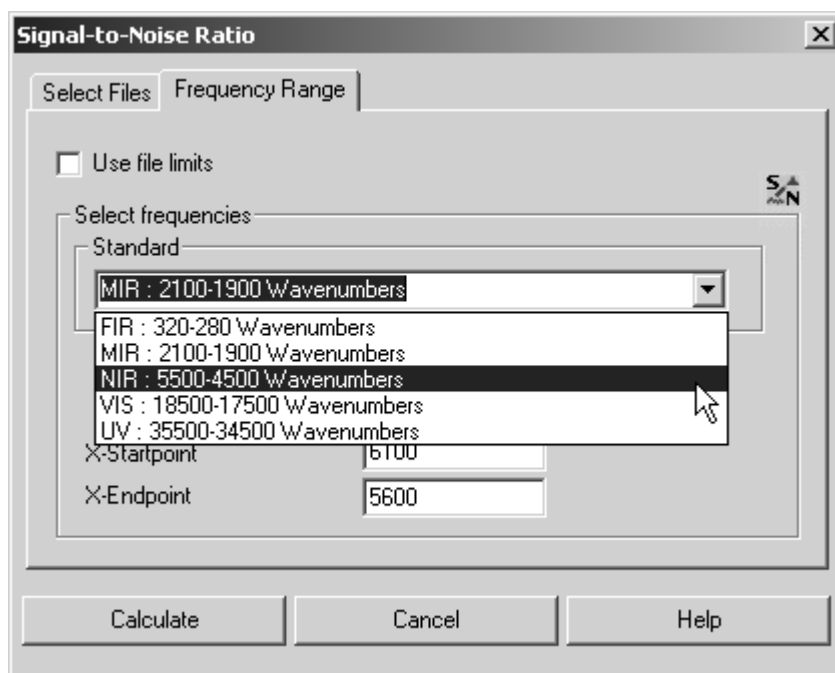
Figure 150: Signal-To-Noise-Ratio - Frequency Range

3.7.5   Peak Picking

Definition	The *Peak Picking* command allows to identify maximum (absorption spectrum) or maximum (transmission spectrum) peaks of a spectrum.
Principle	OPUS uses a standard method which is generally used for peaks with small or no overlapping in spectra. This method is especially recommended in case of low or average spectral resolution (0.5cm^{-1} or above).

To perform peak picking...

... see chapter 2.1.4.

Interactive peak picking

1   Load a spectrum file.
2   Select the *Peak Picking* command from the menu.
3   The following view is displayed:
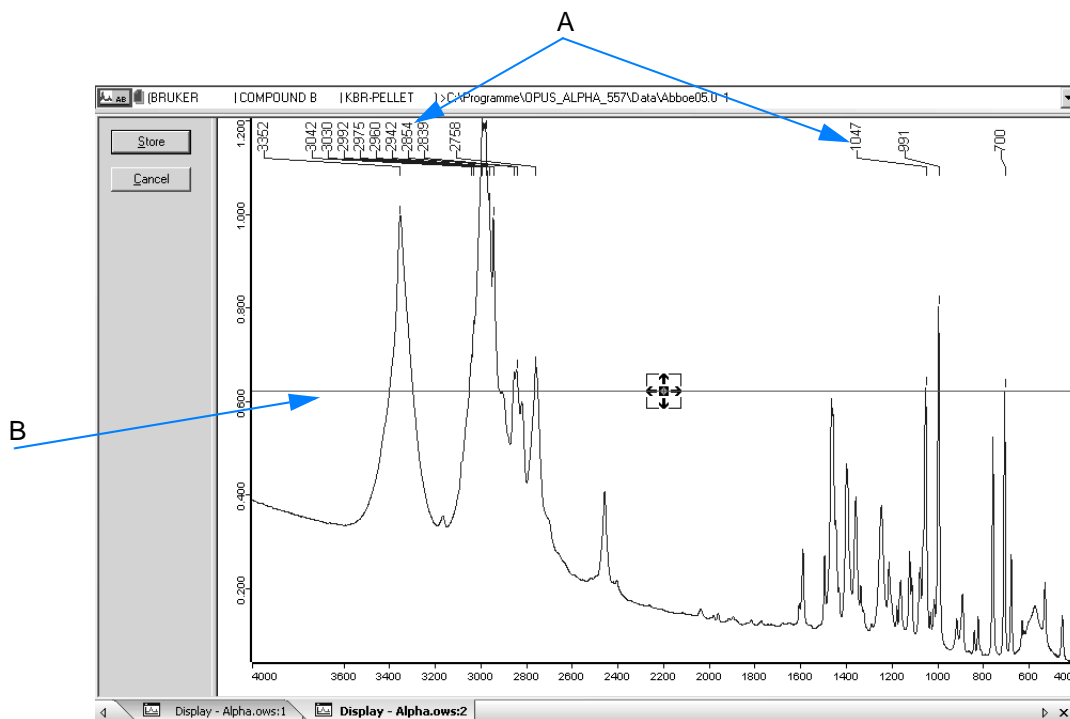
Figure 151: Interactive Peak Picking

4   By default, a maximum peak sensitivity is set, i.e. a as many as possible number of peaks are displayed (A in figure 151).

5   A line (B) is shown by default which can be moved upwards and downwards to define a certain threshold value for peak picking.

Note: In some applications very small bands may be neglected, and in other cases high-intensity peaks are normal and thus the low-intensity peaks may be crucial. Therefore, specify the threshold value for peak picking by moving the line.

6   To move the line left click on the line point and move the line upwards or downwards. **Note: If the threshold has been changed, only those peaks will be displayed which are above (absorption spectrum) or below (transmission spectrum) this line.** To remove the line from the view, just double click on the line point.
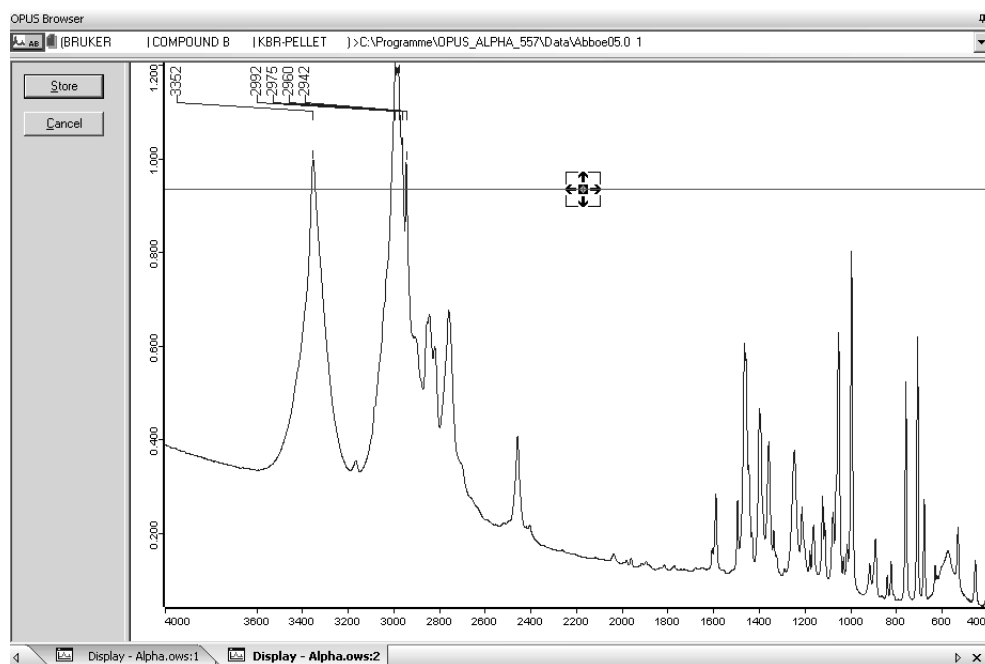
Figure 152: Interactive Peak Picking - Absorption spectrum
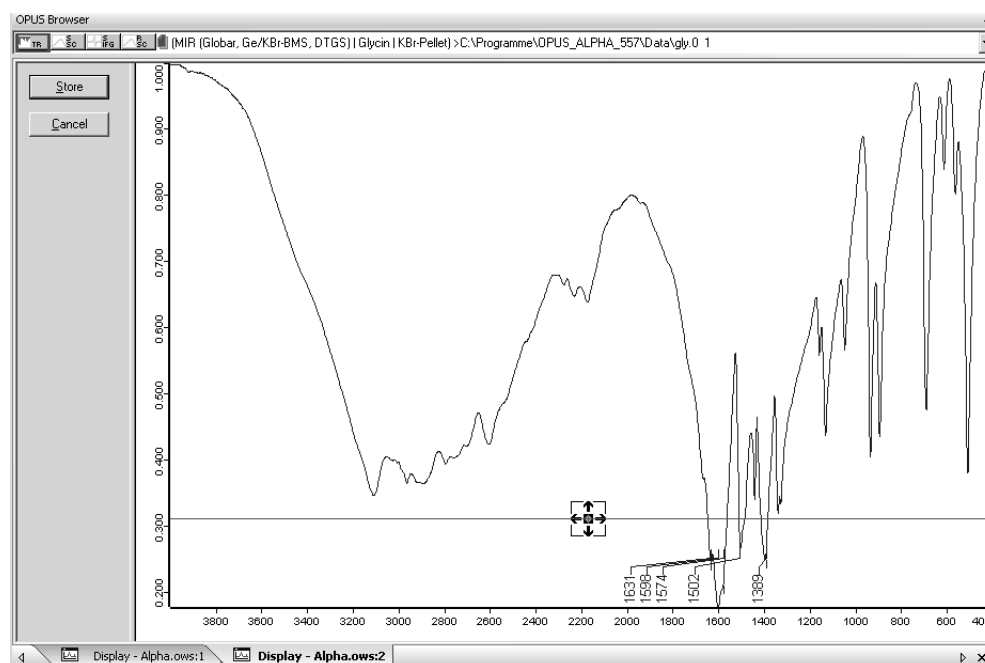
Figure 153: Interactive Peak Picking - Transmission spectrum

7   To store the interactive peak picking click on the *Store* button. The view closes and the spectrum window is displayed again.

The peak picking result...

...is stored in the ⌠PEAKS⌡ data block. The peak parameters are displayed in the *Info* view below the spectrum window.
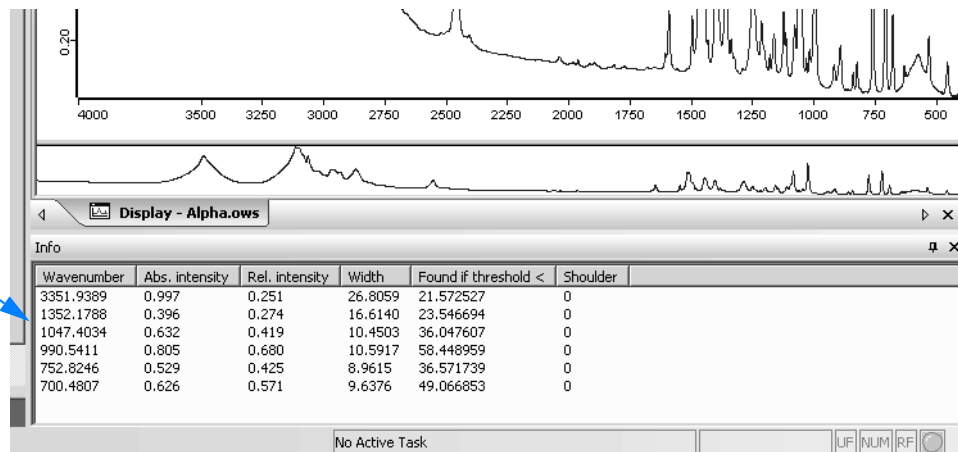
Figure 154: Peak picking result

To display the peak picking result in a report window...

...right click on the ⌠PEAKS⌡ data block in the browser and select the *Show Peak List* option from the pop-up menu.

The report window opens and contains the name and date of the sensitivity as well as the number of bands.
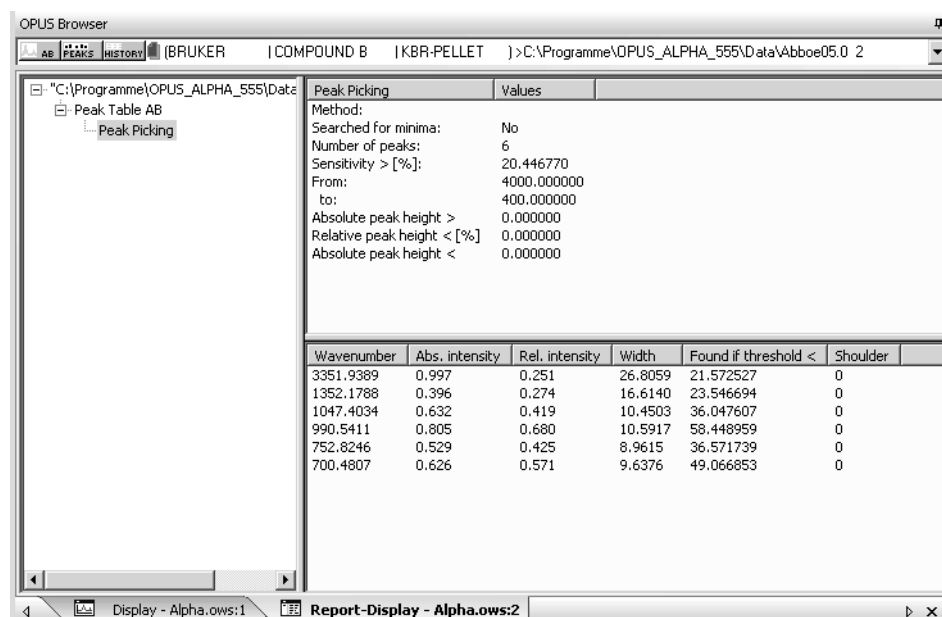
Figure 155: Peak Picking - Report window

3.7.6   Quick Compare Setup

Definition	This command allows to create a method for quick compare (see chapter 3.7.7).
Principle	To create a quick compare method at least one reference spectrum or several reference spectra are required. Reference spectra are made of samples which meet certain quality requirements. See also chapter 2.2

To create a method...

1   ...select the *Quick Compare Setup* command.

2   A dialog opens. Click on the *Reference Files* tab and select the respective spectrum files.

3   Click on the *Parameters* tab to make further settings.

4   Store the method on the *Load/Store Method* tab.

Note: Creating or editing a quick compare method requires administrator rights in OPUS.

The different tabs are described in the following in the order as described above.

Reference Files
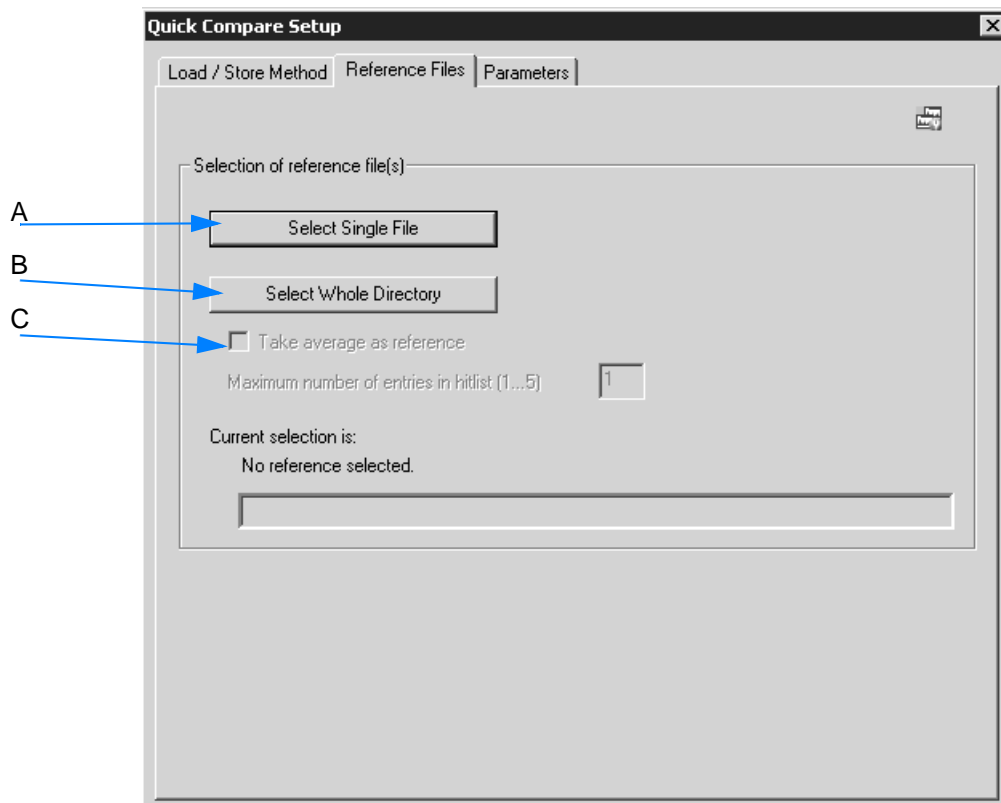
Figure 156: Quick Compare Setup - Reference Files

A You can either select one single spectrum file or...

B ...several spectra files of a complete directory. **In both cases a dialog opens from which you select the file(s).**

C If you have selected a complete directory, the *Take average as reference* check box will be enabled.
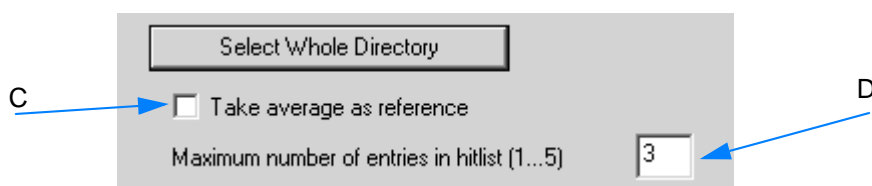
If you activate this check box (C), an average reference spectrum will be calculated from all spectra stored in the directory currently selected.

D To perform the comparison with all reference files, define the maximum number of entries to be included in the hit list. Up to 5 entries are possible.

The path of the directory or spectrum currently selected will be displayed below *Current selection*.

Current selection is:

Whole directory

C:\Programme\OPUS_ALPHA_555\
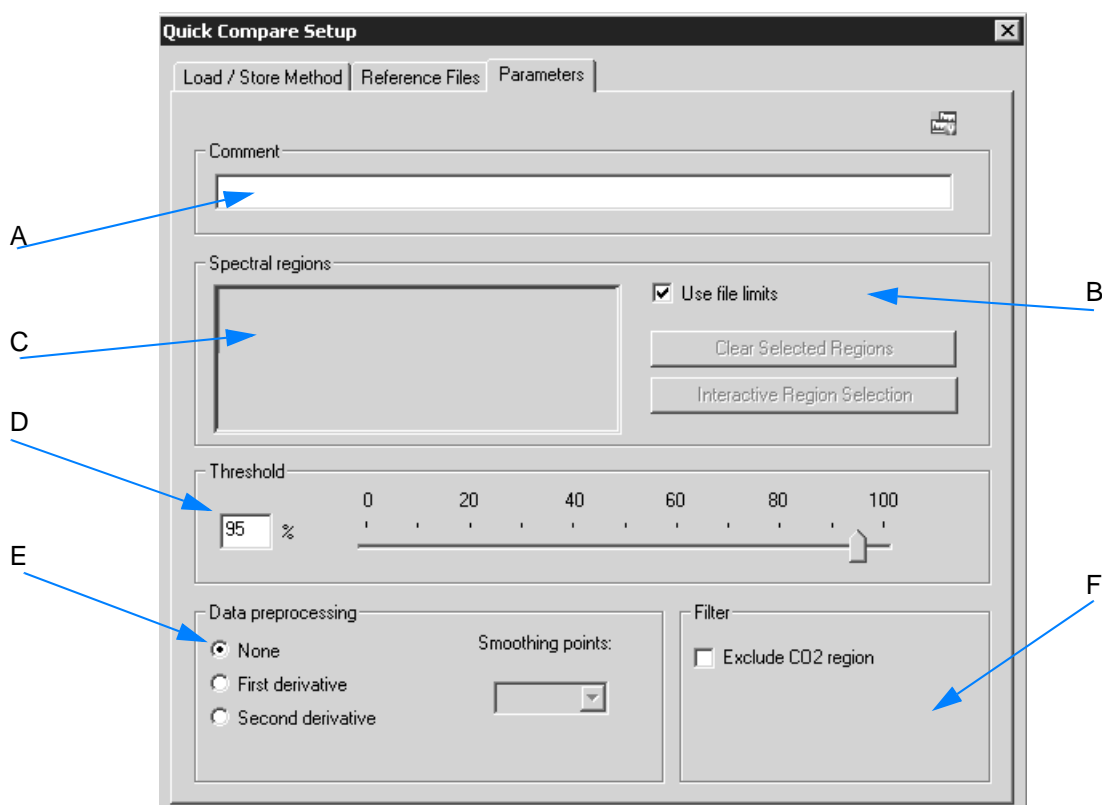
Parameters

Figure 157: Quick Compare Setup - Parameters

A The *Comment* entry field can be used to enter any kind of text, e.g. details about the method created, e.g. *Two spectral regions*, *No data preprocessing* etc.

B The *Use file limit* check box is activated by default. This means that the wavenumber range is based on the first - and possibly only - reference spectrum. If you deactivate this check box, the *Interactive Region Selection* and *Clear Selected Regions* buttons as well as the *Spectral Regions* table will be enabled.

C To select the spectral regions you can either manually type the limits into the table or select them interactively. In the latter case click on the *Interactive Region Selection* button.

Move the borders of the frequency region, or right click into the frequency region and select one of the options from the pop-up menu. For detailed information on the pop-up menu refer to chapter 1.13.1.

If you want to delete one or more spectral region(s), select the respective line(s) on the *Spectral Regions* table and click on the *Clear Selected Region*s button. To delete the spectral regions when working in interactive mode right click on the region and select the *Remove* option from the pop-up menu.

D Use the slider to determine the threshold, i.e. the degree of similarity between the reference and sample spectrum. The threshold determines whether the quick compare result is OK. The result is OK, if the correlation coefficient (see chapter 3.7.7) is greater than the threshold selected.

The result is not OK if the correlation coefficient is less than the threshold selected. You can also manually enter the exact threshold value between 0 and 100% into the corresponding entry field.

E Optionally, you can select between three different data pre-processing methods. If you check the *First* or *Second Derivative* option button, the *Smoothing Point* selection box will be enabled. The optimal number of smoothing points set for the specific pre-processing methods has to be determined empirically.

F The *Exclude CO_2 Region* check box allows to exclude CO_2 bands from the calculation. If you activate this check box, the wavenumber regions of 660 to 680cm^{-1} and 2,275 to 2,400cm^{-1} are excluded when calculating the correlation coefficient.

Load/Store Method
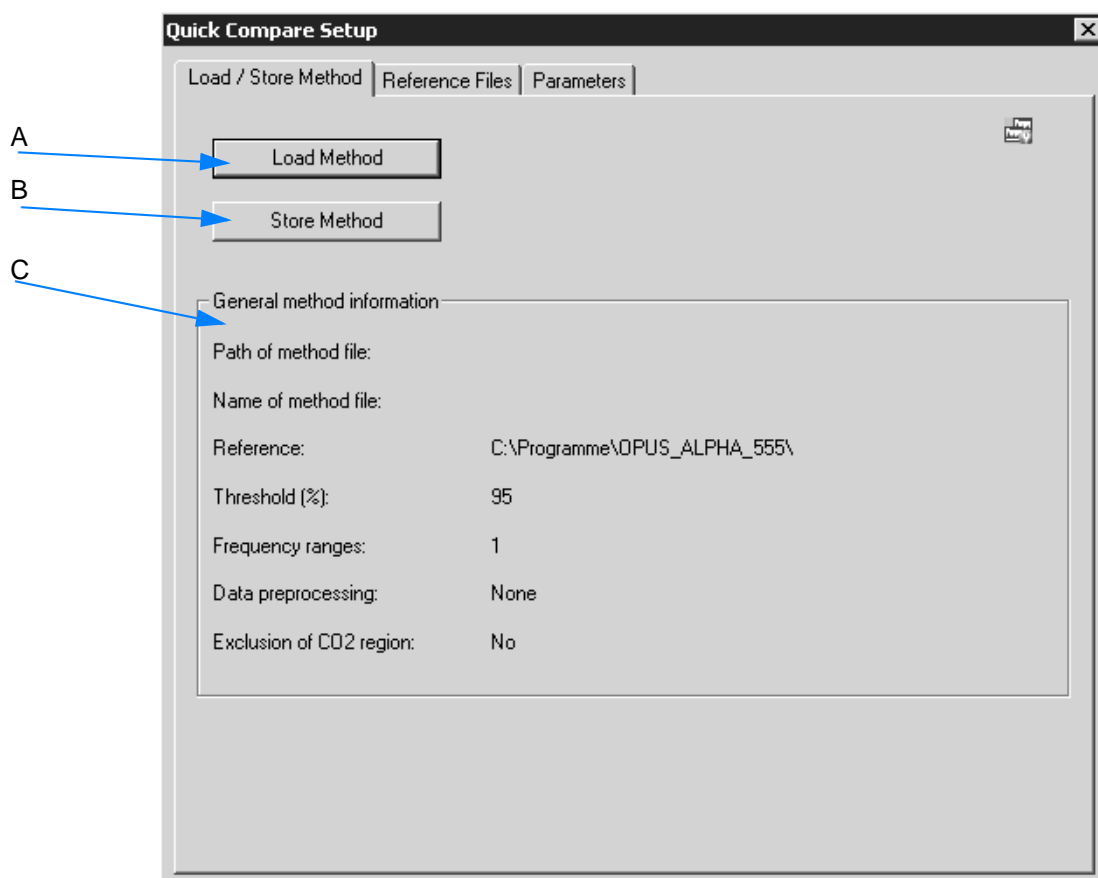
Figure 158: Quick Compare Setup - Load/Store Method

A To load an existing method click on the *Load Method* button. Select the respective method from the dialog that opens.

B Click on the *Store Method* button to store the new method. This button is only enabled if you have specified a reference file and a wavenumber range before.

C The *General method information* group field includes information on the method, e.g. path and method file name, threshold, data preprocessing etc.

The Quick Compare method...

...has the file extension *.QCM*.

3.7.7   Quick Compare

Definition	The *Quick Compare* command is a quality control tool. Loaded sample spectra files are compared with one reference spectrum file, or several reference spectra files of a complete directory. A a correlation coefficient is calculated.
Principle	The spectrum files used for Quick Compare have to include either an AB (absorption) or TR (transmission) data block. Quick Compare parameters are stored in a special method file, see chapter 3.7.6.

Basic Features

The comparison between sample and reference spectrum will be performed by calculating the correlation coefficient.

The correlation coefficient *r* of the two functions $y_1(k)$ and $y_2(k)$ is calculated as ratio from the covariance and product of the two standard deviations σ_{y_1} and σ_{y_2}:

$$r = \frac{Cov(y_1(k), y_2(k))}{\sigma_{y_1} \cdot \sigma_{y_2}}$$

The value of *r* ranges between -1 (inverted spectra) and +1 (identical spectra). This correlation coefficient *r* will be calculated into a percentage and reflects the similarity of the two spectra. The $-1 \leq r < 0$ range is mapped to 0%, and the $0 < r \leq 1$ range is mapped linearly to 0% ...100%.

How to perform Quick Compare?

1   Load the spectrum file to be compared.
2   Select the *Quick Compare* command.
3   The *Quick Compare* dialog opens and automatically includes the name of the spectrum file in the *File(s) for Quick Compare* selection field.

   Note: Make sure that the data blocks for the sample and reference files are of the same spectra type, i.e. AB (absorption) or TR (transmission). Besides, the wavenumber range of the sample spectrum has to be at least as large as the range defined for the reference spectra.
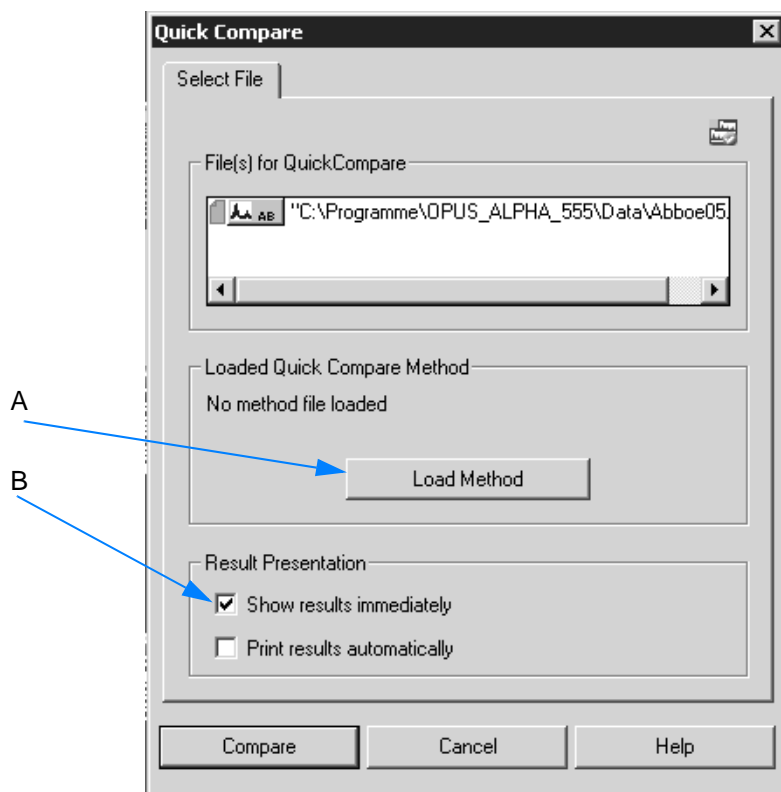
Figure 159: Quick Compare - Select File

4   Load a method by clicking on the *Load Method* button (A in figure 159). Select the method from the dialog that opens.

Note: If a method has been loaded, the name and path of the method is displayed.
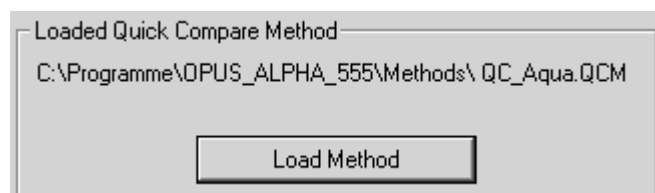
5   By default, the *Show results immediately* check box is activated. The result is shown in a special result view immediately after Quick Compare has been completed.

6   Click on the *Compare* button to perform Quick Compare.

The Quick Compare result...

...is stored in the ![icon] data block and displayed in a separate result view.

Quick Compare result view
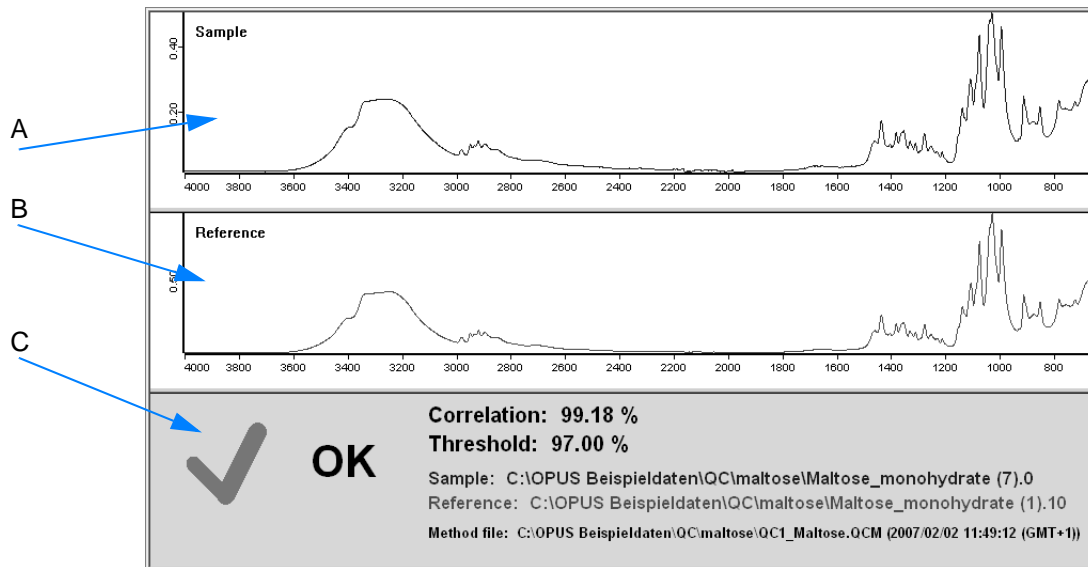
Figure 160: Quick Compare with one reference - result OK

A Sample spectrum

B Reference spectrum

C Quick Compare result, the following results are possible:

- **Green check mark and *OK*:** the comparison has passed. In this case the correlation value calculated is greater than the threshold value defined in the method.

- **Red cross and *Not OK*:** the comparison has failed. In this case the correlation value calculated is less than the threshold value defined in the method.
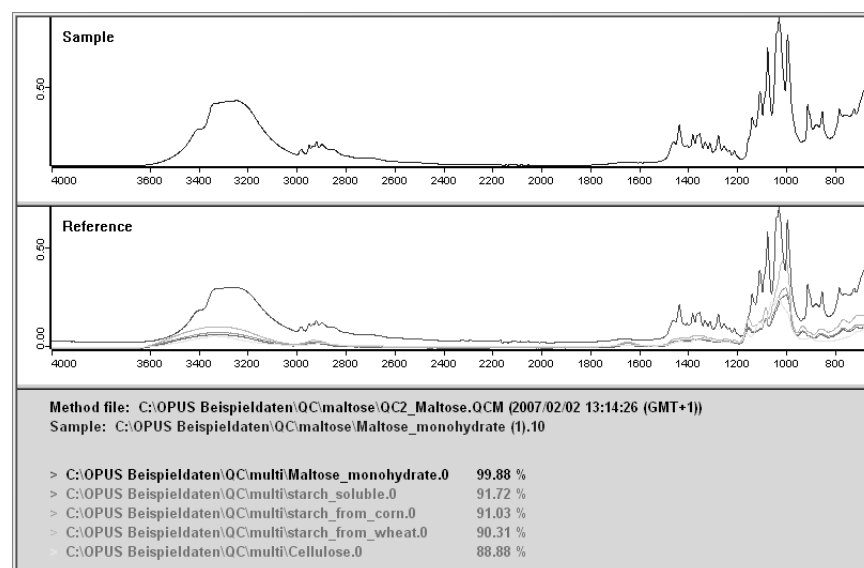
Figure 161: Quick Compare with several references - 1 hit found

For further information on the *Quick Compare* result views refer to chapter 2.2.

To display the Quick Compare result in a report window...

...right click on the ⟨≈ QC⟩ data block in the browser and select the *Show Report* option from the pop-up menu.

The report window opens and contains the correlation coefficient as well as the number of hits found.
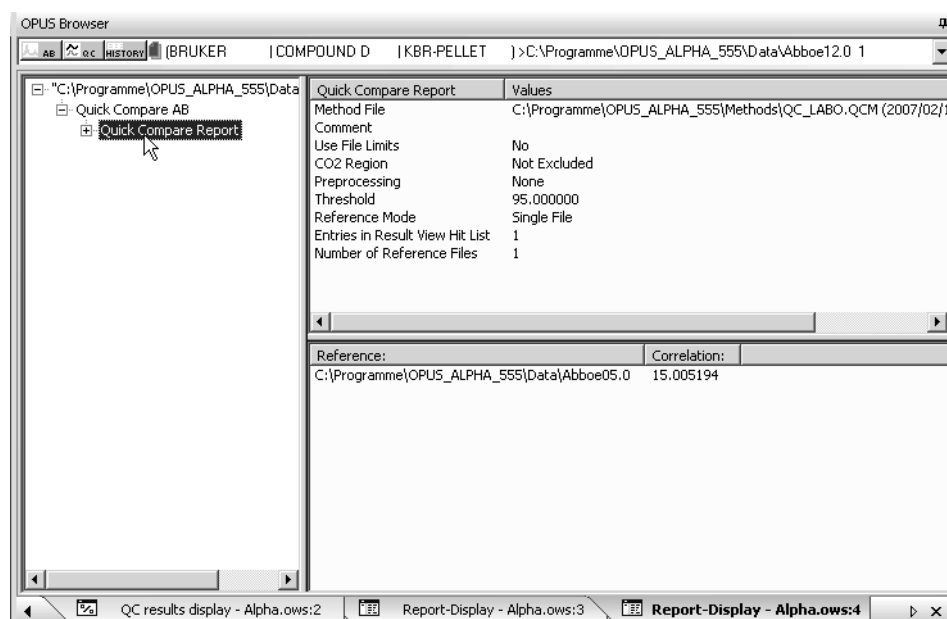
Figure 162: Quick Compare - Report window

3.7.8   Spectrum Search 🔎

Definition	The *Spectrum Search* command allows to identify an unknown spectrum by comparing it to spectra from a library. Library spectra which show distinct similarities to the unknown spectrum are detected and listed in a search report.
Principle	There are two kinds of demonstration libraries available in OPUS: • DEMOLIB.SO1 • SR.IDX The libraries are stored in the OPUS path: *<OPUS>\DATA\-LIBRARY.* When using the *Spectrum Search* command transmission spectra will automatically be converted into absorption spectra to get a reasonable result. However, both the query spectrum and the search results will be displayed in transmission.

To perform Spectrum Search...

1   ...load a spectrum file.
2   Select the *Spectrum Search* command. The *Spectrum Search* dialog opens.
3   Specify the search parameters and define the regions by means of the single dialog tabs.
4   Select the libraries you want to work with.
5   Start spectrum search by clicking on the *Search Library* button.

Note: For detailed information on spectrum search by means of the wizard refer to chapter 2.3.

The different tabs of the *Spectrum Search* dialog are described in the following.

Spectrum Search
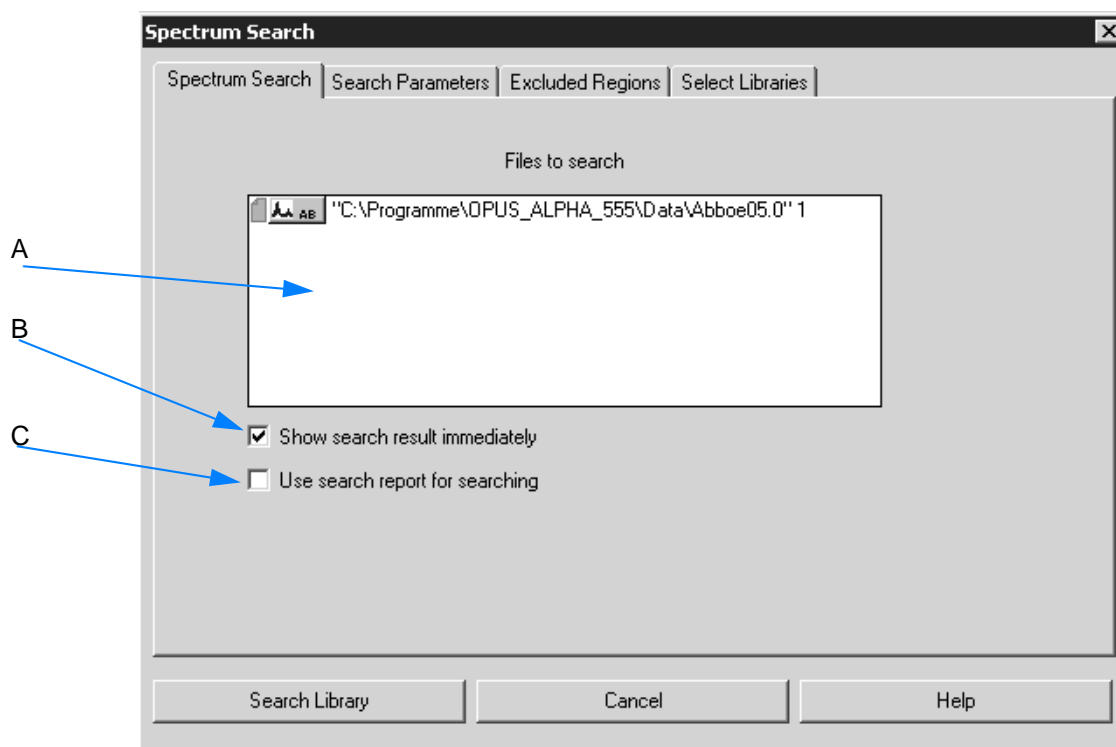
Figure 163: Spectrum Search

A If you have loaded a spectrum file and selected the *Spectrum Search* command, the name and path of the spectrum file loaded is automatically displayed in the selection field.

B If you activate this check box, the result view is automatically shown after spectrum search has been completed. For further details on this view refer to the information given in this chapter or in chapter 2.3.2.

C If you activate this check box, a small field opens below the check box from which you can select an already existing search report. **Note: In this case the search will not be performed by means of the settings made on the *Select Libraries* tab, but only by those spectra which are included in the search report. This enables to refine a search previously performed.**

Search Parameters

Three different search algorithms are available which are described in the following.

- **Standard**

A
B
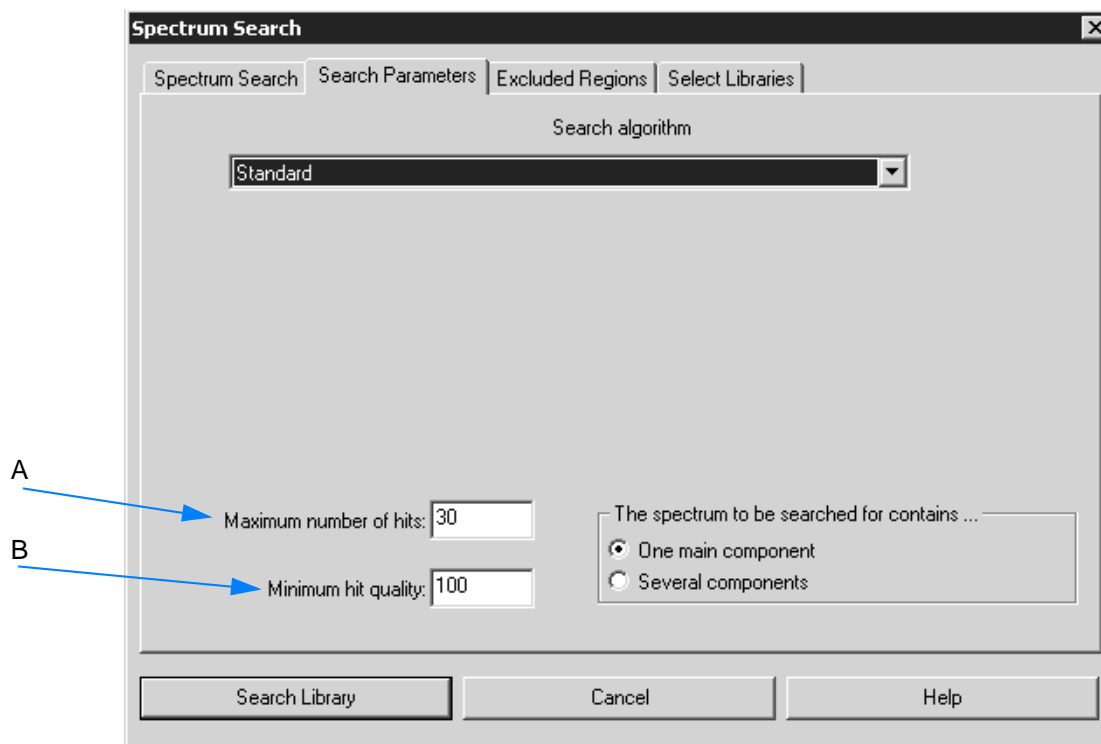
Figure 164: *Standard* search parameter

In case of the *Standard* search algorithm all pieces of band information, which are available from the query and library spectrum, are reflected in the hit quality. This kind of information contains:

- the position,
- relative intensity and
- half-width

of each band. A library spectrum band is considered to be identified in the query spectrum if this spectrum contains a band

- which position does deviate from the position in the library spectrum by less than the half-width,
- which difference between the half-widths and relative intensities is less than factor 2, respectively.

This algorithm also allows to further specify the search result. Select the appropriate option button to define whether the query spectrum consists of one main component or multiple components.

A This setting specifies the maximum number of hits that are to be saved in the search report.

B This setting specifies the minimum hit quality required for a hit to be saved in the search report. A hit quality of 1000 would be a perfect conformity, whereas a value of 0 is obtained if there is no correlation at all. In general, the search algorithm produces a value of >0 even if there are no or negligible similarities between spectra. Therefore, it is reasonable not to include all hits below a certain limit (default setting: 300) into the search report.

As the minimum hit quality also depends on the data acquisition method it first should be evaluated by measuring reference samples. Only if such a search yields no hits should you set the minimum hit quality to a lower value.

- **Use existing peak table**
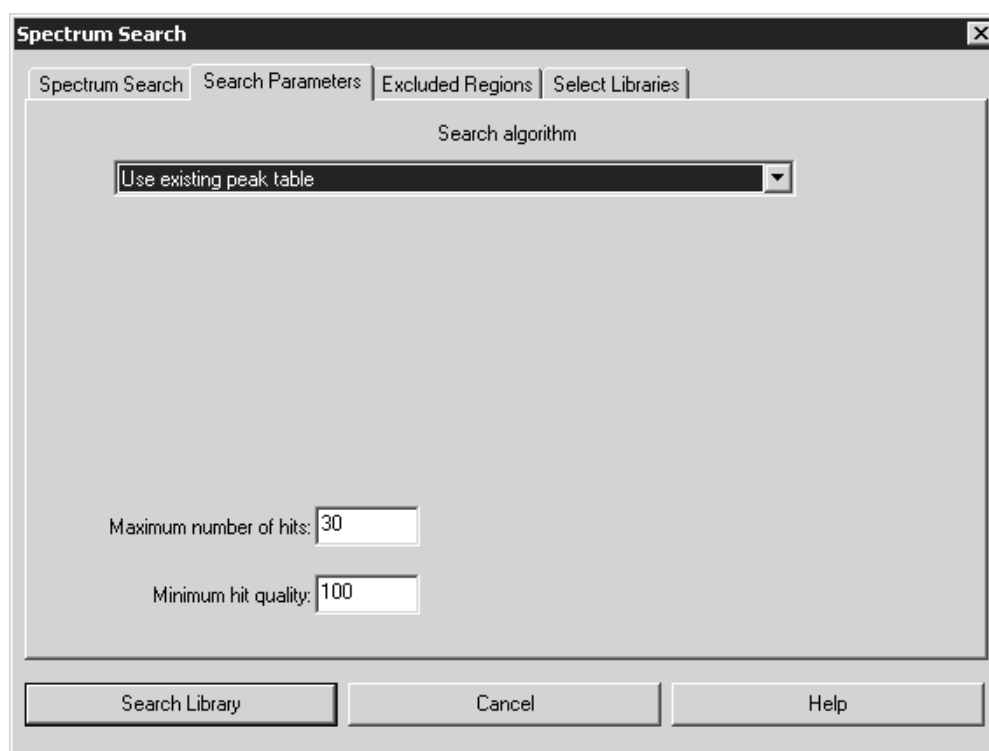
Figure 165: *Use existing peak table* search parameter

This algorithm uses an already existing peak table, which enables you to suppress the influence of peaks originating from the substrate.

- **Spectrum correlation**
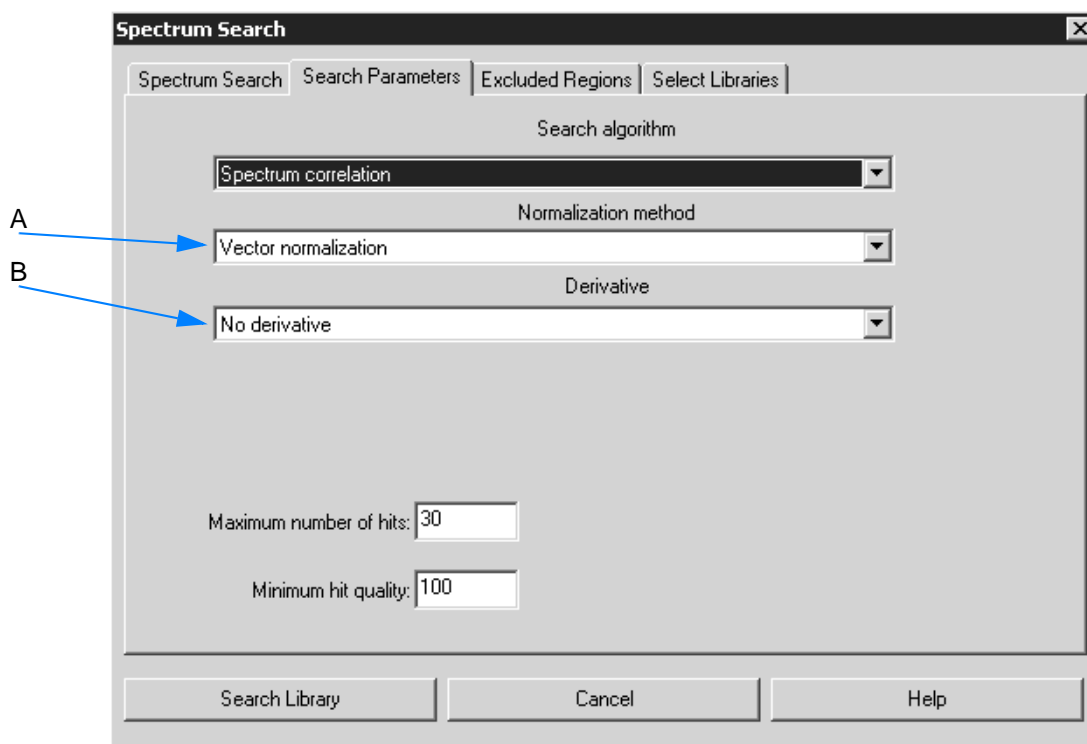
Figure 166: *Spectrum correlation* search parameter

The *Spectrum correlation* algorithm calculates the sum of the squared deviations between the query spectrum and the result spectrum for the data points of the range defined. The summation can be limited to a spectral range selected by the user.

A Select an appropriate normalization method. The following methods are available.

  - **Vector normalization**

    The vector normalization data preprocessing normalizes a spectrum, i.e. the average *y* value is calculated first and subsequently subtracted from the spectrum. Then, the sum of squares of all *y* values is calculated and the spectrum is divided by the square root of this sum.

    This method is used in case of different optical thickness to compare the samples with each other. The form of the different spectra will be preserved, which facilitates the interpreting of spectra. However, the result extremely depends on the spectral region selected, i.e. specific differences of one region are distributed to all data points.

  - **Min-Max normalization**

    This method scales spectrum intensities to the effect that the minimum of each spectrum will be 0 and the maximum 1.

B Select an appropriate derivative. The following types of derivative are available:

- **No derivative**
- **First derivative**

  Calculates the first derivative of the spectrum by interpolation. Steep edges of a peak become more important compared to flat structures.

- **Second derivative**

  The second derivative is similar to the first derivative and additionally allows to evaluate extremely flat structures.

Excluded Regions
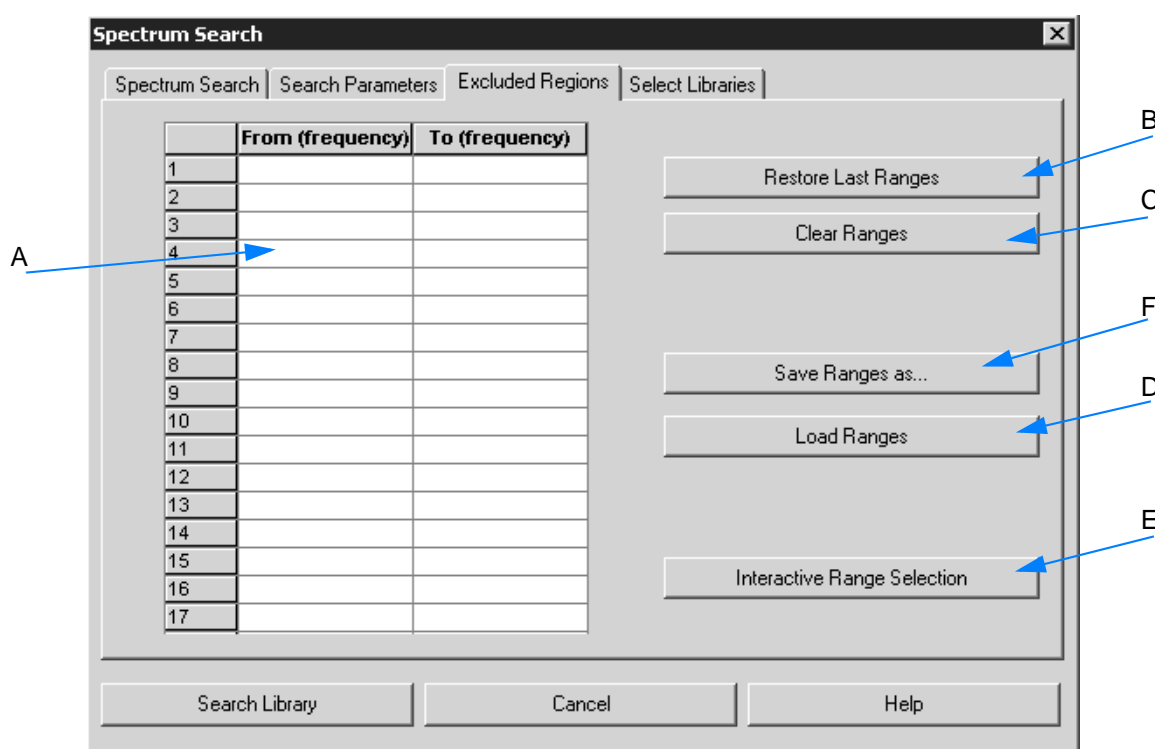
Figure 167: Exclude regions

There are several possibilities to define the regions you want to exclude.

A You can manually enter the ranges into the table. To delete single lines only, click on the respective line number and press the *Del* button on the PC keyboard.

B If you want to use the frequency ranges of the previous search run, click on the *Restore Last Ranges* button.

C Sometimes it may be advisable to delete CO_2 bands from an MIR spectrum. Click on the *Clear Ranges* button to delete the table entries and enter the new ranges you want to use for the next query.

D To load an already existing data set click on the *Load Ranges* button.

E To interactively select the frequency ranges, click on the *Interactive Range Selection* button. A window opens and displays the query spectrum.

Right-click on the spectrum and select the *Add Region* button from the pop-up menu. The spectral ranges to be excluded are displayed on a white background. If you position the cursor on the edges of the spectral ranges and press the left mouse button, you can re-size the ranges.

F If you have completely filled in the table, store the data set by using the *Save Ranges as* button.

Select Libraries

You have to define one or more libraries to be used for spectrum search. A search can involve either one or more libraries, but creates only one search report in either case.
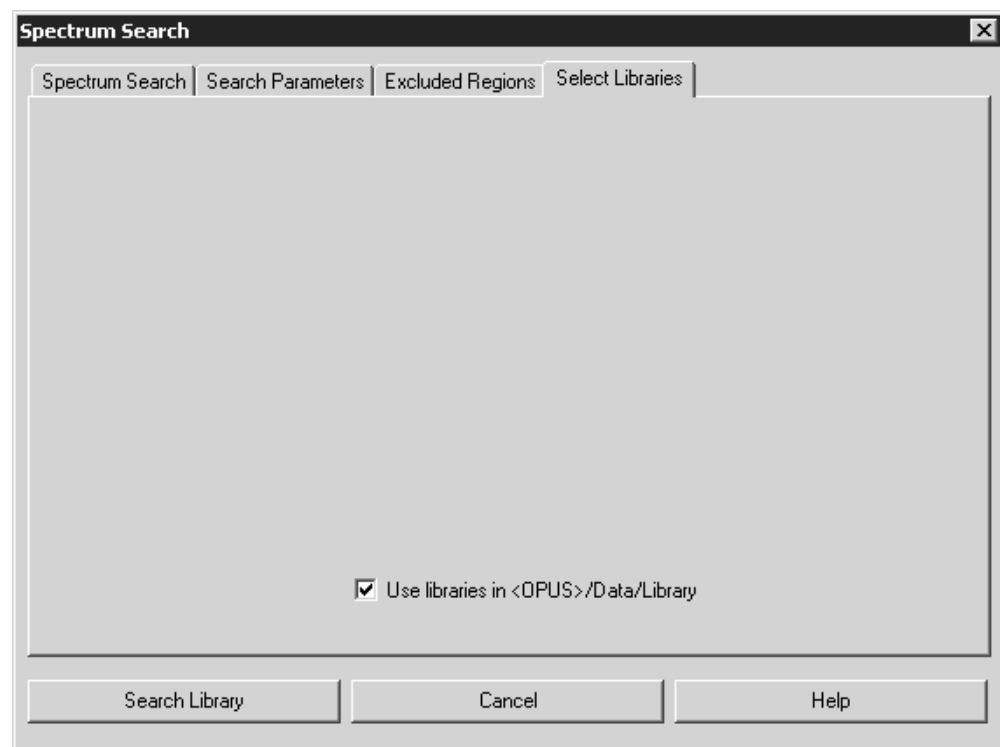
Figure 168: Using standard OPUS libraries

By default, the *User libraries in OPUS/Data/Library* check box is activated. If you deactivate this check box, the *Select Libraries* tab changes as follows:
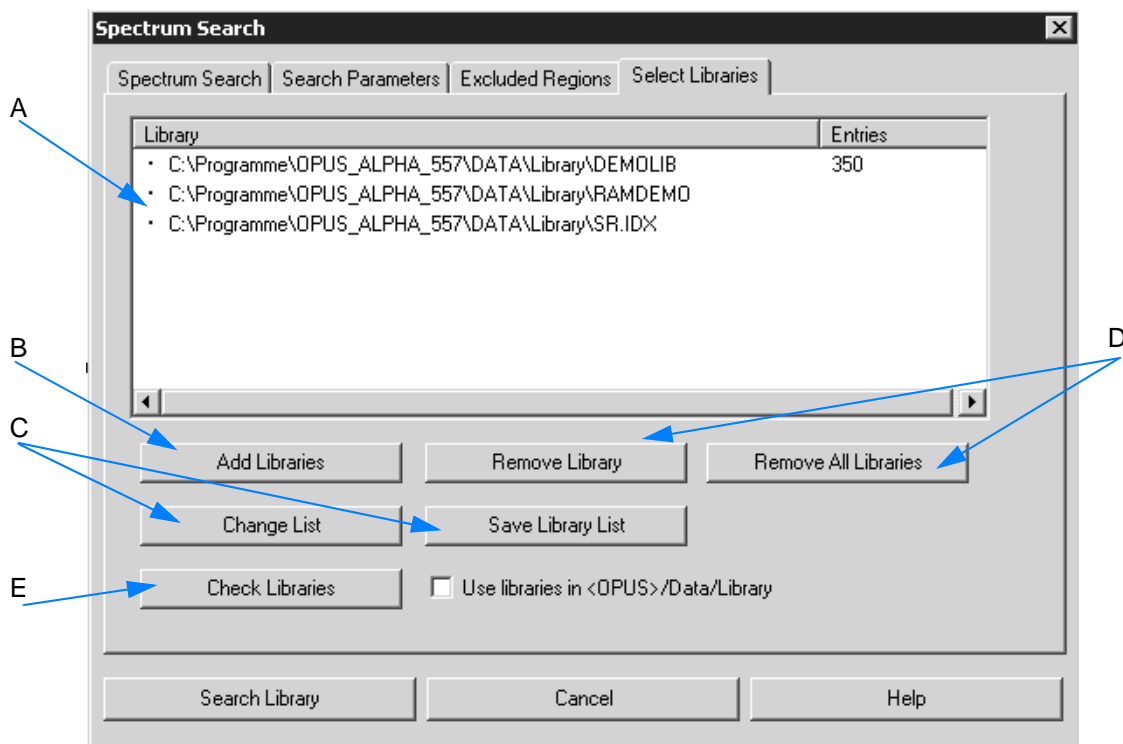
Figure 169: Selecting libraries

A The selection field contains the libraries selected for spectrum search.

B Use the *Add Libraries* to add a different library into the selection field (A).

C Save a library created by means of the *Save Library List* button. To modify a library click on the *Change List* button. The library previously used will be set by default the next time when using the *Spectrum Search* command.

D To delete single libraries select them in the selection field (A). Click on the *Remove Library* button. To delete all libraries click on the *Remove all Libraries* button.

E You can also check the library status by clicking on the *Check Libraries* button. The following types of status are possible:

- **Black point:** library not checked

- **Green check mark:** library is okay

- **Red exclamation mark:** error in library

- **Red cross:** library has not been found; this may occur, if the library has been deleted or the directory changed. If the library status has been checked, the number of library entries are indicated.

Figure 170: Different types of library status

Note: If you want to load a library from CD, insert the CD into the CD drive, and keep the CD in the drive during the search run.

The spectrum search result...

...is added to the query spectrum in the form of the ⊞SEARCH data block and displayed in a separate result view.

The spectrum search result view...

...is immediately shown after spectrum search has been completed, provided you have activated the *Show search result immediately* check box (B in figure 163 on page 165).

If you have not activated this check box, left click on the ⊞SEARCH data block in the browser to open the spectrum search result view.
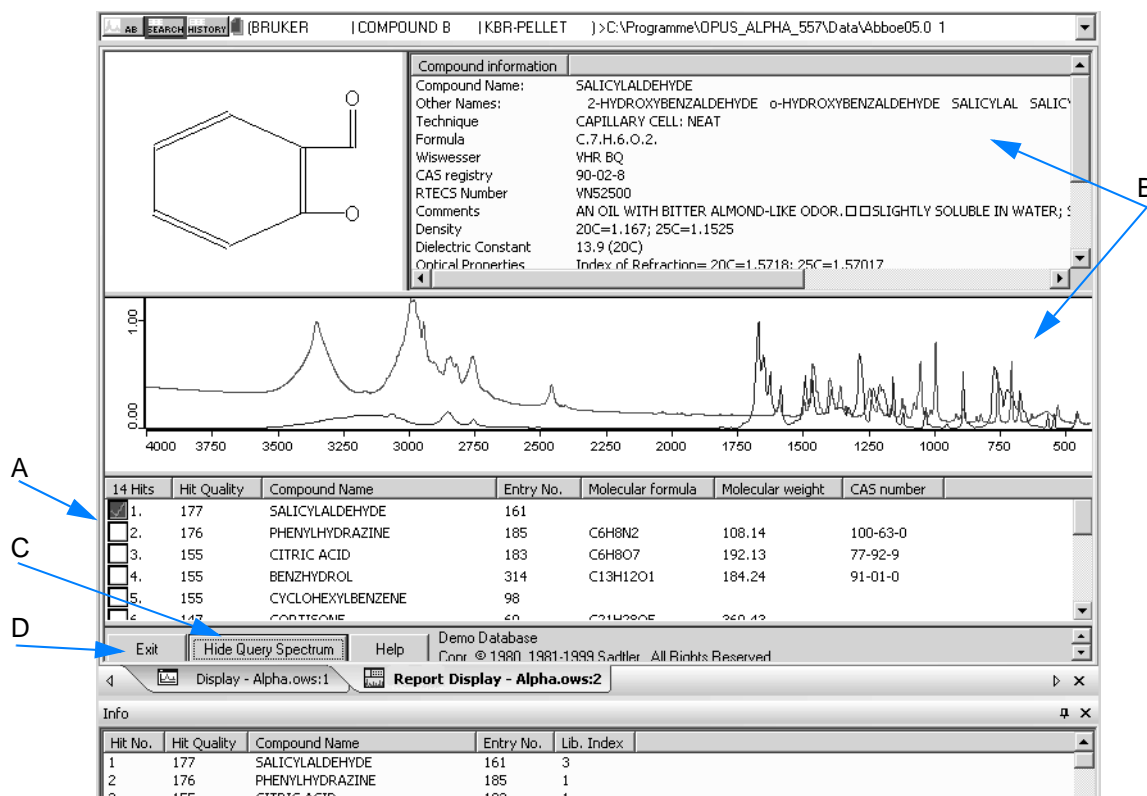
Figure 171: Spectrum search result view

The result view consists of four different windows which can be re-sized by moving the window frames.

A This window includes the total number of search hits ranked according to their hit quality. Additional features of the hit list are the compound name as well as the entry number. Generally, the first hit is automatically checked and...

B ...its spectrum is displayed, together with the structural formula and compound information. The lower window also contains the query spectrum.

C If you click on the *Hide Query Spectrum* button, only the hit spectrum is displayed. If you have clicked on the *Hide Query Spectrum* button, the button will change into *Show Query Spectrum*. Spectra are automatically displayed in transmittance, if the query spectrum is a transmittance spectrum.

D To close the result view click on the *Exit* button.

3.7.9   Initialize Library

Definition	The *Initialize Library* command allows to create and edit libraries in OPUS format.
Principle	There are two possibilities to create a library: • adding spectra files to new library • creating empty library

3.7.9.1   Adding spectra files to new library

1   Load the spectra files.

2   Select the *Initialize Library* command. The following dialog opens:
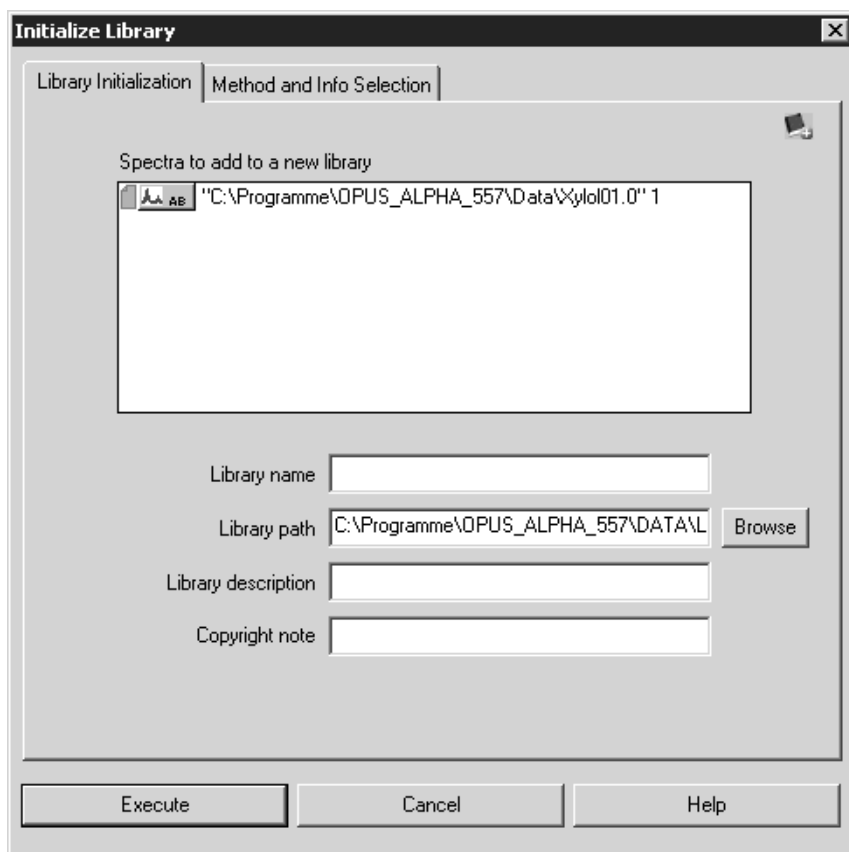
Figure 172:   Add spectra to library

3   By default, only one spectrum file of those loaded is shown in the *Spectra to add to a new library* selection field. Drag & drop the remaining spectra files from the browser into the selection field. **Note that only ratio data blocks, e.g. AB or TR will be accepted.**

4　Fill in the different entry fields. If you click on the *Browse* button, you can change the default library path.

5　Click on the *Execute* button to create the library.

Note: When creating the library according to the procedure described above, the library parameters will be derived from the first spectrum displayed in the selection field. This is the reason why all functions on the *Method and Info Selection* tab are completely deactivated.

3.7.9.2 Creating empty library

1　Select the *Initialize Library* command.

2　Click on the *Method and Info Selection* tab.

3　Define the settings, e.g. which kind of spectra information of each spectrum has to be added to the library.

4　Click on the *Execute* button.

The *Method and Info Selection* tab, with the different options available, is described in the following.
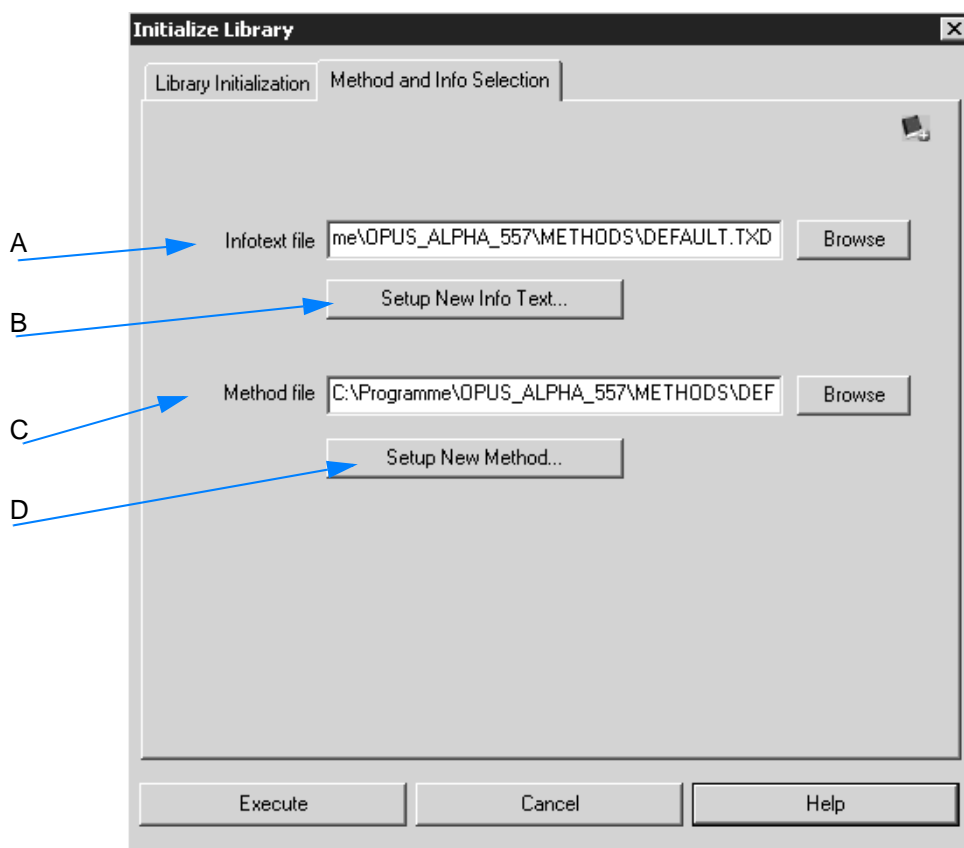
Figure 173: Creating empty library

A The info text file determines which kind of information mask is used to have the spectra information (INFO) displayed. If you click on the *Browse* button, you can load an existing info text file. **Info text files have the file extension *.TXD.**

B To create a new info text file, click on the *Setup New Info Text* button. For further details see below.

C A method file defines the frequency range and digital resolution of spectra used for the library to be created. **Method files have the extension *.MTD.** If you click on the *Browse* button, you can load an existing method file.

D To create a new method click on the *Setup New Method* button. For further details see below.

Setting up new info text

Click on the *Setup New Info Text* button (B in figure 173). The following dialog opens:
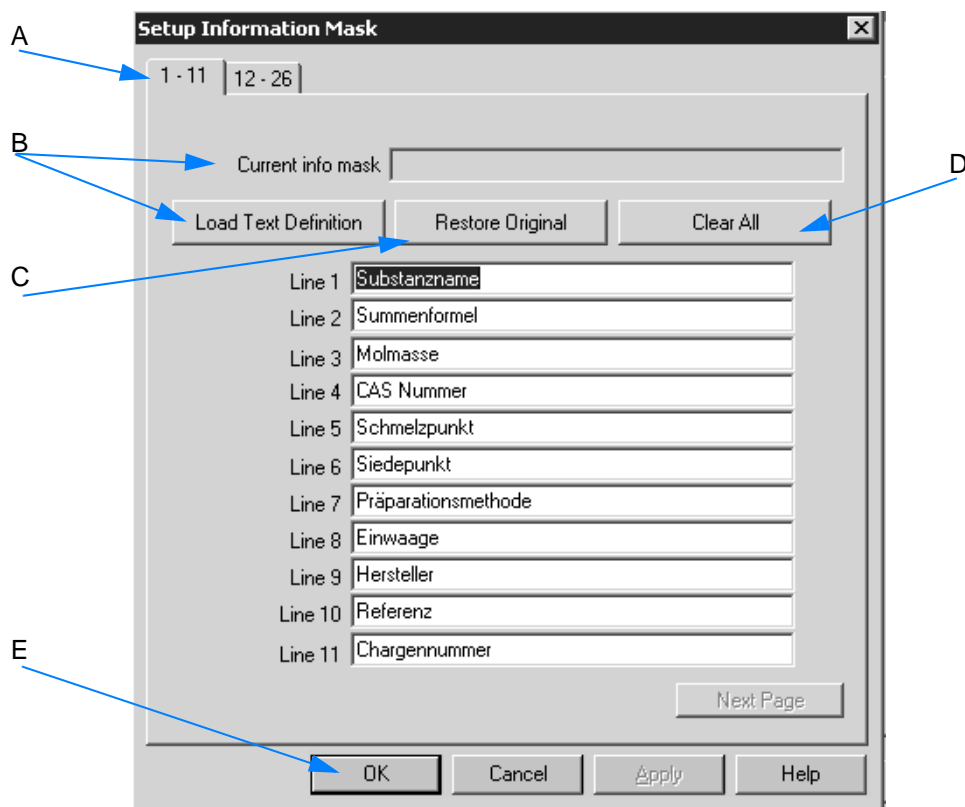
Figure 174: Setup Information Mask

A The two tabs *1-11* and *12-26* indicate the number of lines displayed in the mask.

B If you click on the *Load Text Definition* button, you can load an existing info mask which you can use as template. By default, the following info masks are available under *<OPUS>Method*:

- Default.txd
- extended.txd

As soon as you have loaded an info mask the name and path of this mask is displayed in the *Current info mask* field.

Current info mask　C:\PROGRAMME\OPUS_ALPHA_557\METHODS\
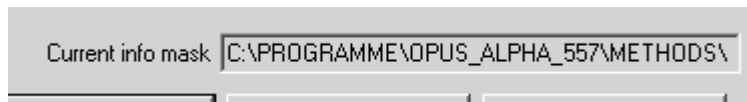
C　If you click on the *Restore Original* button, the original settings of the template will be restored.

D　If you click on the *Clear All* button, all entries in the different lines will be deleted. The lines will be colored red. To enter text just click into the respective field and write the text.

Line 1　Substance
Line 2

E　To store the newly created text mask click on the *OK* button. The *Save File* dialog opens. Define the name of the text mask. After saving the text mask the *Method and Info Selection* tab (figure 173) will be displayed again.

Setting up new method

Click on the Setup New Method button (D in figure 173). The following dialog opens:
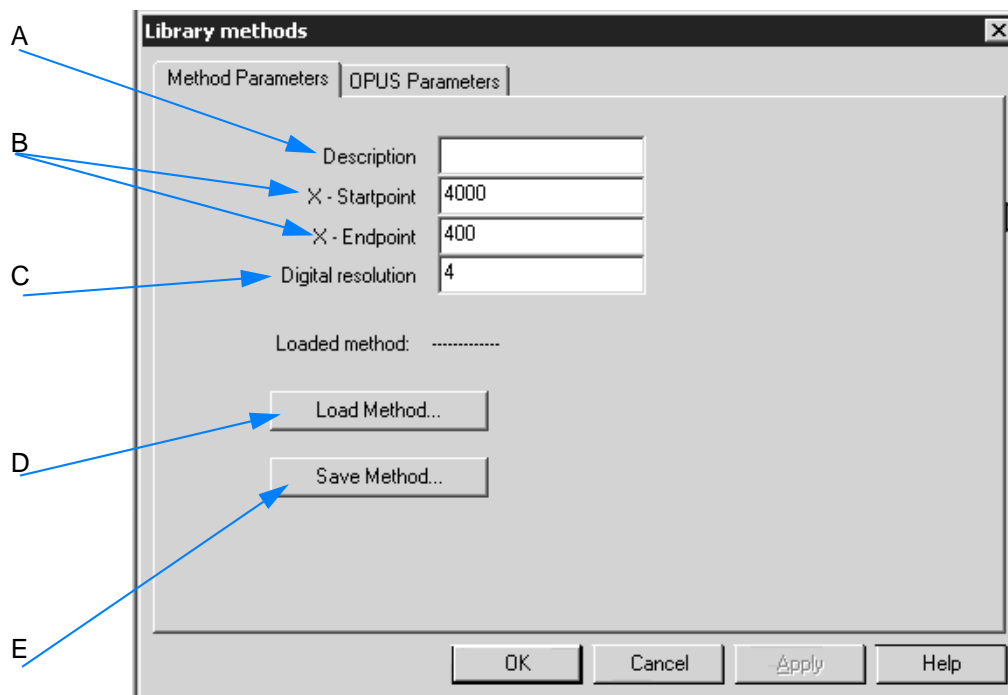
Figure 175: Library Methods

A Define a description for the method.

B Specify the frequency ranges (x-startpoint, x- endpoint).

C Enter the digital resolution of the library spectra. The digital resolution determines the number of data points required to save spectra by using the current method. This feature has a direct effect on the space needed by the library on the hard disk. As a rule of thumb, in case of a library using the Default method (4,000 - 400cm^{-1}, digital resolution 4cm^{-1}) you can anticipate a disk space of about 6 - 7Mbyte per 1,000 spectra.

Note: The digital resolution refers to the spectra saved which are used for correlation algorithms, display, plot and - in case of mixtures - subtraction. However, the digital resolution does not have any influence on the quality of spectrum searches for the standard algorithm.

If you want to differentiate very identical spectra and if you depend on the correlation algorithm, we recommend a digital resolution of 2 or 1.

D You can also load an existing method file. Click on the *Load Method* button.

E To store the newly created method click on the *Save Method* button. If you do not store a method file created, the *Save File* dialog automatically pops up as soon as you click on the *OK* button.

On the *OPUS Parameters* tab you define the parameters which are to be stored with each spectrum available in the library.
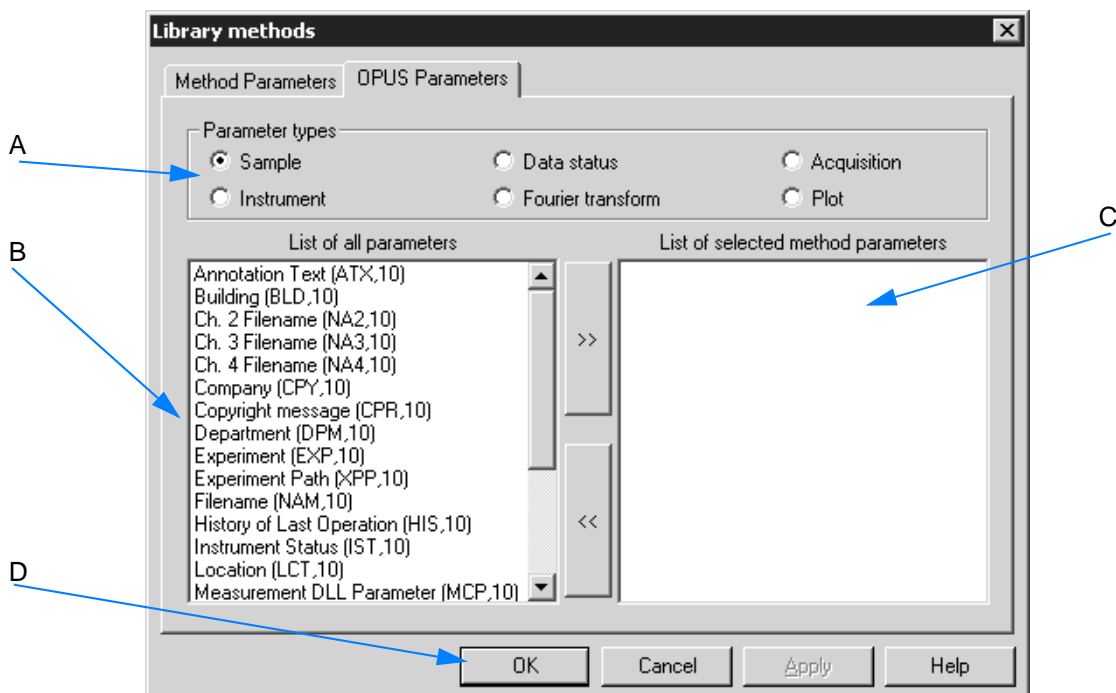
Figure 176: Selecting OPUS parameters

A The parameters have been grouped into different types. You can switch between these types by clicking on the respective option buttons.

B The *List of all Parameters* selection field shows all parameters available, depending on the parameter type selected (A). To select a particular parameter left click on it and move it to (C) by using the arrow button.

C The *List of selected Method Parameters* selection field only includes the parameters selected for the library.

D If you click on the *OK* button, the *Save File As* dialog pops up. Define the name of the method. After saving the method the *Method and Info Selection* tab will be displayed again (figure 173). Clicking on the *Execute* button on this tab creates a new library.

3.7.10 Store Spectrum in Library

Definition	Spectra files can be stored into an existing library.
Principle	To get reasonable search results the spectra to be stored should only be absorption or transmission spectra. If you use transmission spectra, they will be converted into absorption spectra and also saved as absorption spectra.

To store a spectrum file into a library...

1.   ...load the respective spectrum file.
2.   Select the *Store Spectrum in Library* function.
3.   Define the parameters on how the spectrum is to be stored in the library.
4.   Click on the *Store* button.

The different tabs of the *Store Spectrum in Library* dialog are described in the following.

Store Spectrum
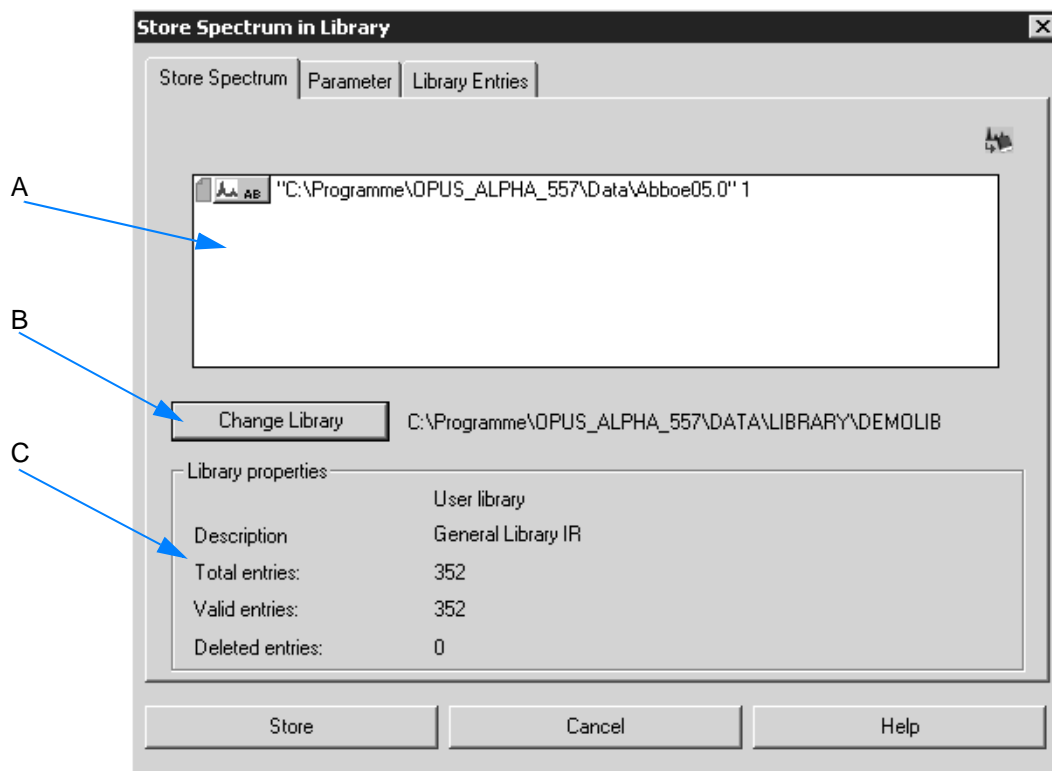
Figure 177: Store spectrum file

A By default, only one spectrum file of those loaded is shown in the *Spectra to add to a new library* selection field. Drag & drop the remaining spectra data blocks (AB, TR) from the browser into the selection field. If a warning symbol is displayed on the *Store Spectrum* tab, the data block does not match the settings made on the *Parameters* tab.
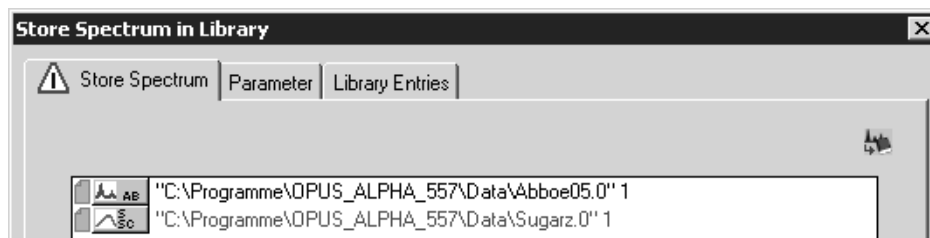
Note that the option buttons checked on the *Parameters* tab for a previous operation will automatically be selected by default. If the name and path of the spectrum file is displayed in red in the selection field, the file will not be added to the library.

B The *Change Library* button allows to select a different library to be used to store the spectra. Select the respective library from the dialog that opens.

C The *Library properties* group field identifies the library currently selected. The library description entered during the setup will also be displayed, together with some library statistics.

Parameter
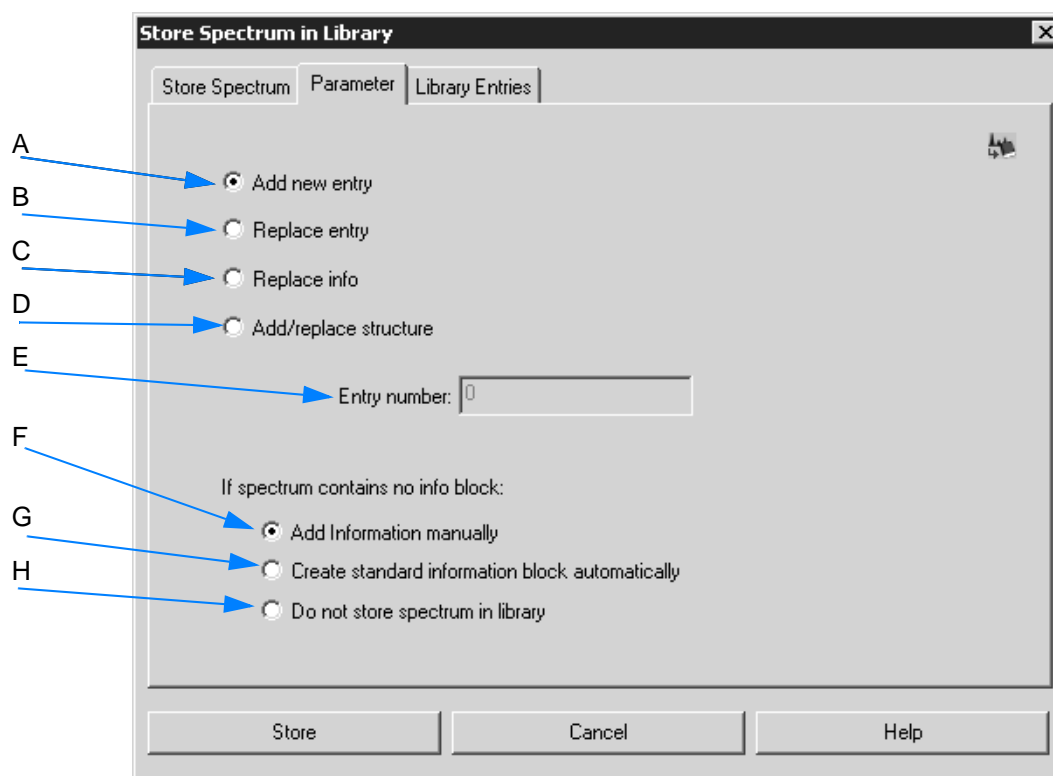
Figure 178: Defining parameters

A If you check the *Add new entry* option button, the spectrum will be added to the library.

B If you check the *Replace entry* option button, the existing library entry will be replaced by a new one. **Make sure that you have specified which entry you want to replace. Enter the corresponding entry number into the *Entry Number* field (E).**

C If you check the *Replace info* option button, the info text only of an existing library entry will be replaced.

D If you check the *Add/replace structure* option button, the chemical structure formula of the spectrum is added or replaced. **Make sure that you have specified which entry you want to replace. Enter the corresponding entry number into the *Entry Number* field (E).**

E The entry field is only enabled, if you check the options buttons (B) and (D). Enter the number of the respective entry into the field.

F You can define how to proceed with spectrum files which do not have an INFO data block (⊞ INFO). If you check the *Add Information manually* option button and click on the *Store* button, you will be prompted to enter the relevant spectra information.

G To automatically create an INFO data block select the *Create standard information block automatically* option button. **This kind of INFO data block is based on the sample parameter data avail-**

> **able for the sample name, sample type, and operator. This
> data block is stored in the library together with the spectrum.**

H If you check the *Do not store spectrum in library* option button, all
spectra which do not contain an INFO data block will NOT be
stored in the library.

Library Entries
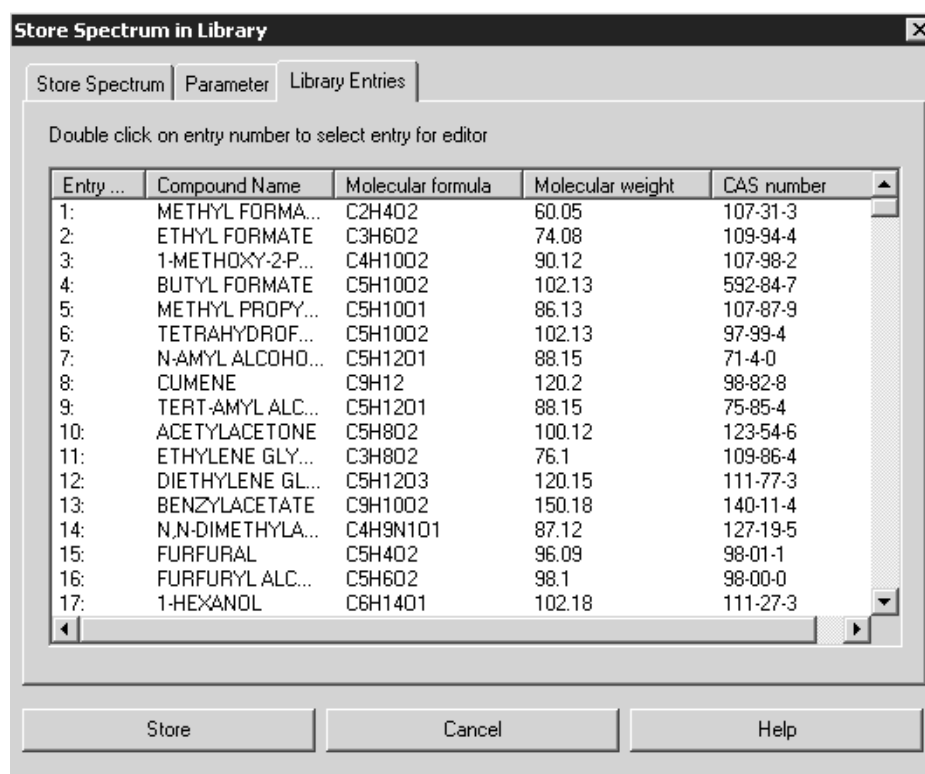
Figure 179: Library entries

The *Library Entries* tab shows the different parameters of all entries. The
parameters include:

- entry number
- compound name
- molecular formula
- molecular weight
- CAS registry number

If you click on a particular column header, e.g. *Compound Name*, the
entire table entries will be sorted in ascending order according to the
column selected. If you click on the particular column header again, the
table entries will be sorted in descending order.

Double clicking on a particular entry automatically transfers you to the
Parameter tab. The number of the entry selected will be shown in the
Entry Number field.

3.7.11 Library Editor

Definition	The library editor allows to administer self-generated libraries, i.e. extract and delete library entries, edit library descriptions and information text.
Principle	Each tab of this command contains different editing features which can be used to change library entries.

How to use the library editor?

1 Select the *Library editor* command.
2 Make the necessary changes.
3 Click on the *Edit* button.

The different tabs of the *Library Editor* dialog are described in the following.

Library Editor
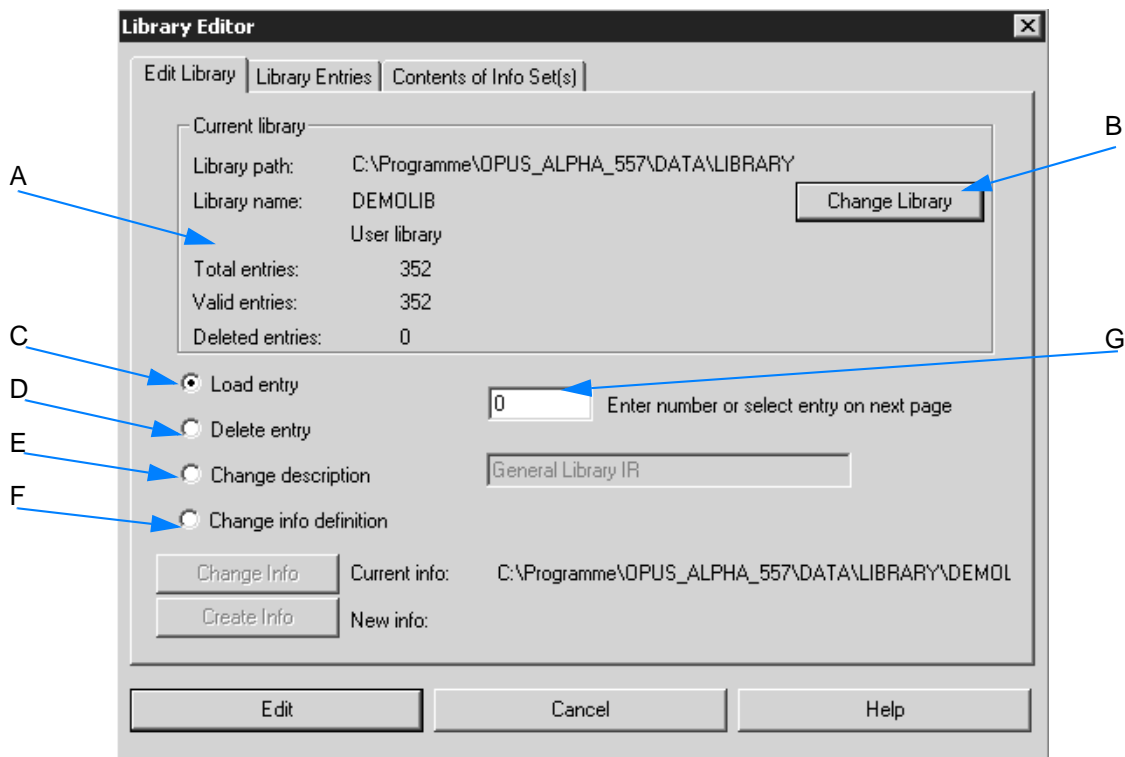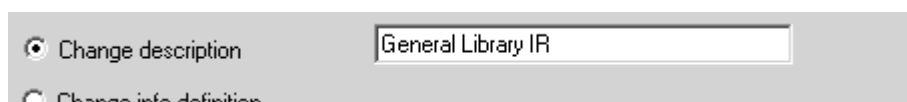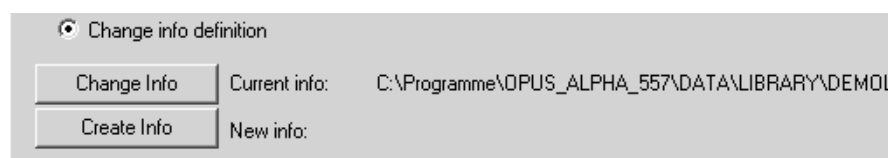
Figure 180: Edit Library

A The *Current Library* group field includes information about the library currently used, e.g. library name, path and description. The total number of entries is also shown as well as the number of valid or deleted entries.

B Use the *Change Library* button to select a different library.

C Check the *Load entry* option button to extract an entry from the library. The entry is stored as spectrum file by the *ENTRYx.0* name, with *x* being the entry number in the library. **Note that you first have to define an entry number (G), either manually or by clicking on the specific entry number on the *Library Entries* tab.**

D Check the *Delete entry* option button to delete an entry from the library. **Note that you first have to define an entry number (G), either manually or clicking on the specific entry number on the *Library Entries* tab.** As soon as you have deleted an entry, the number of entries deleted will be updated in the *Current Library* group field.

E Check the *Change description* option button to change the library description. Enter the new description into the entry field right next to it.

F Check the *Change info definition* option button to change the info mask assigned to a library. The two buttons below will be enabled.

Either select an existing mask by clicking on the *Change Info* button or create a new mask by clicking on the *Create Info* button. For information on how to create a new info mask refer to chapter 3.7.9.2. **The *Change Info Definition* option button should only be checked to append lines to an existing mask or to correct spelling mistakes in an existing mask.**

G The entry field contains the number of the entry to be edited.

Library Entries
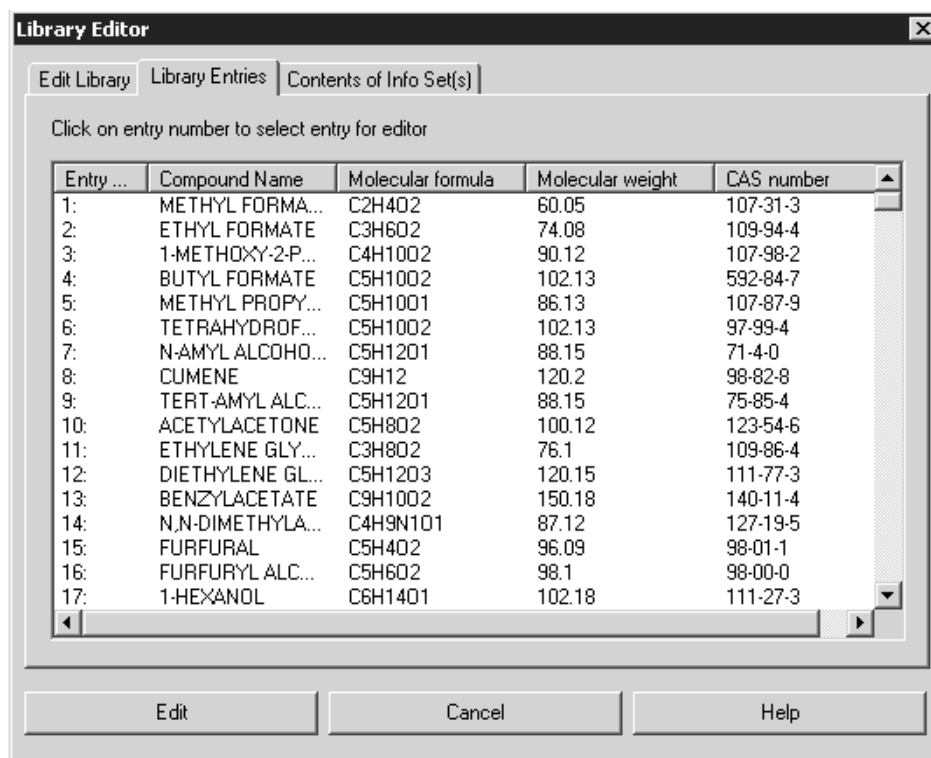
Figure 181: Library Entries

The *Library Entries* tab lists the different parameters of all entries of the library currently used. The parameters include:

- entry number
- compound name
- molecular formula
- molecular weight
- CAS number

If you click on a particular column header, e.g. *Compound Name*, the entire table entries will be sorted in ascending order according to the column selected. If you click on the particular column header again, the table entries will be sorted in descending order.

Clicking on a particular entry number automatically copies the entry number into the destined entry field (G) on the *Library Editor* tab (figure 180) which will be displayed immediately.

When deleting one or more entries from the library...

...this will be indicated next to the particular entry number.
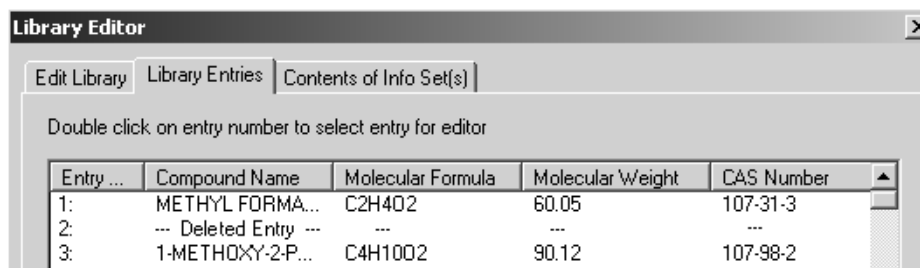
Figure 182: Library entry deleted

Contents of the Info Set(s)
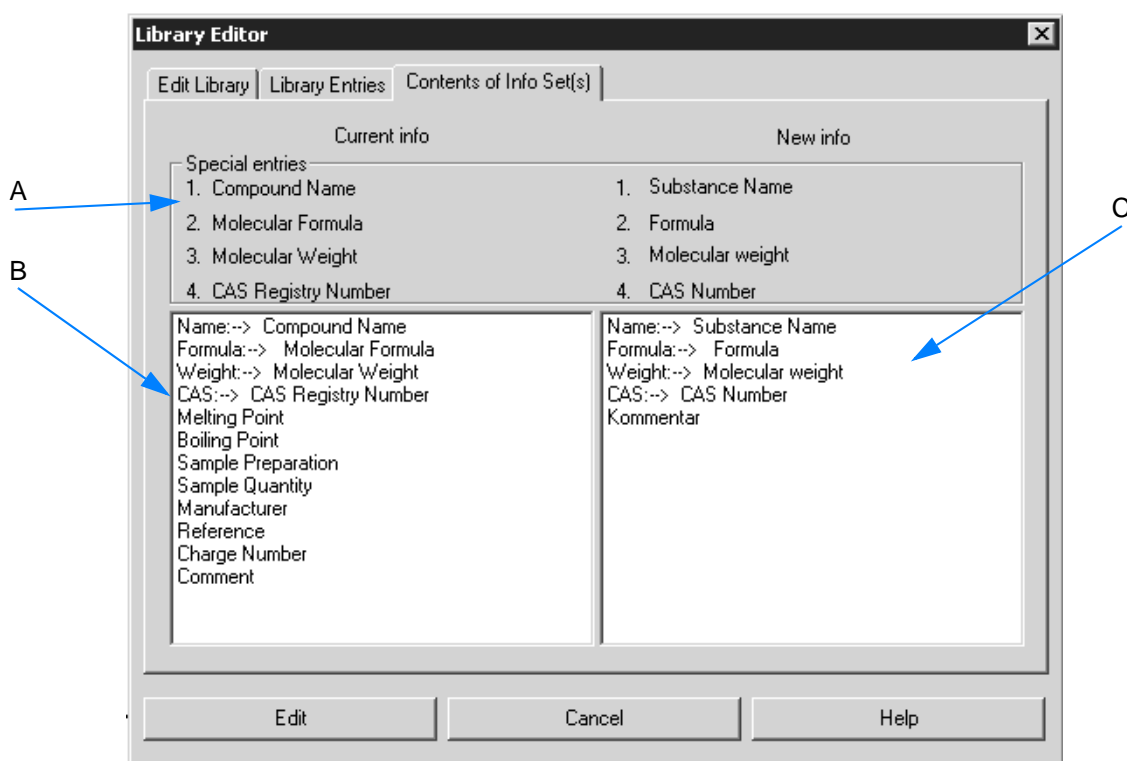
Figure 183: Contents of the Info Set(s)

A The *Special Entries* group field contains the name of the info sets that will be automatically assigned to a library. The corresponding entries are displayed in the respective selection fields.

B The selection field displays the current library info set.

C The selection field displays the info set of the file to be added. The following settings are required before:

a) Check the *Change info definition* option button (F in figure 180).

b) Click on the Change info button (figure 180) and select a new info mask from the dialog that opens. **Info masks have the file extension *.TXD and are normally stored in <OPUS>/Methods.**

c) Click on the *Contents of Info Set(s)* tab.

Thus, it will be easier to see whether the new and the old info mask are compatible. **The new info mask must contain the same entry names - with regard to content - as included in the old one, and may also have additional entries.**

3.7.12 Band Assignment Chart

Definition	The *Band Assignment Chart* command allows to visually assign spectrum bands to functional groups.
Principle	Apart from the functional group name the band assignment chart also includes information on the position and peaks of the bands created by the functional group.
	Wavenumber ranges which may include bands are highlighted by a bar. The bar intensity indicates the band peaks. The less the intensity of the bar, the less pronounced will be the corresponding band.

To open the band assignment chart...

...select the *Band Assignment Chart* command.

The band assignment chart consists of three different windows.
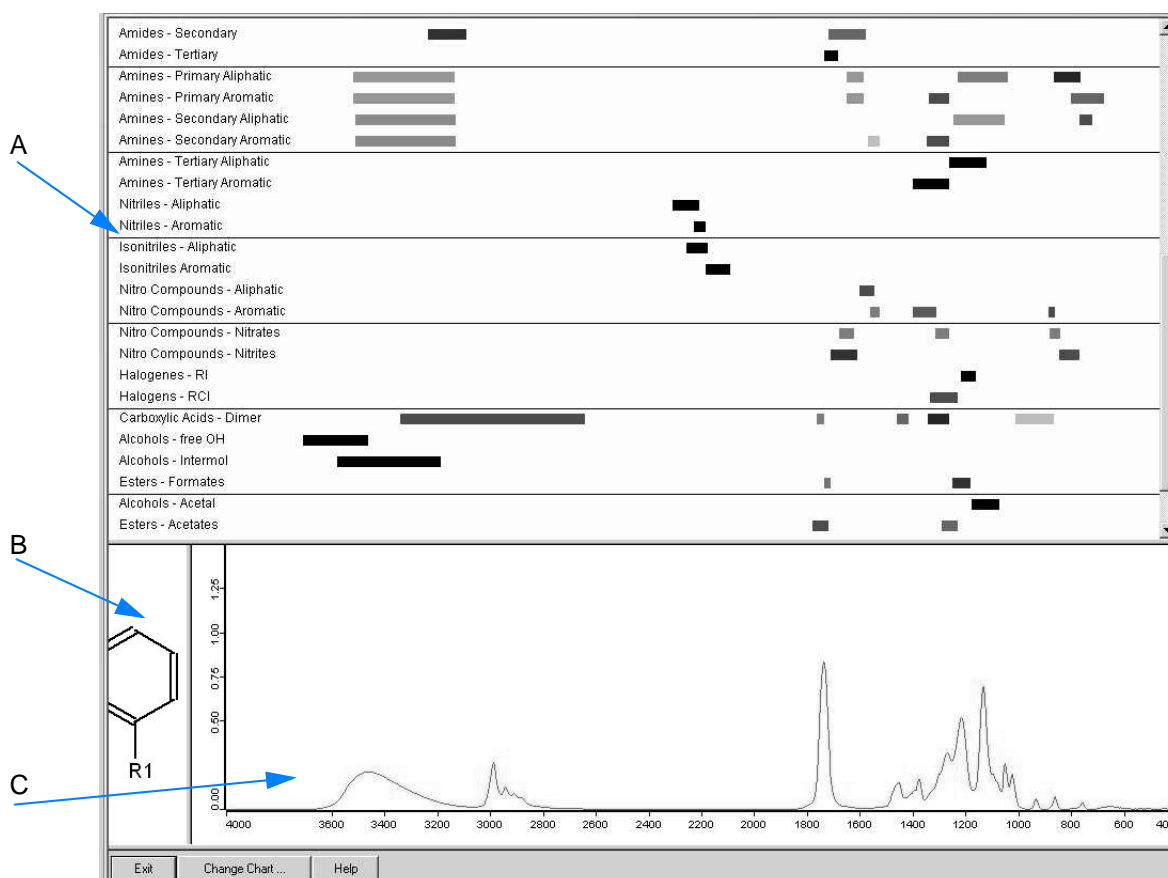
Figure 184: Band assignment chart

A   This window shows a chart which includes the names of the functional groups and their respective band positions in the form of bars.

B   The so-called structure window contains the molecular structure of the functional group selected.

C   The spectrum window shows the spectrum, with the abscissa being always conform with the respective band positions in the upper window (A).

To compare spectra with the band assignment chart...

1   ...load a spectrum file.

2   Select the *Band Assignment Chart* command. The band assignment chart view opens.

3   Drag the spectrum block (▲ AB | or ▼ TR |) of the spectrum file from the browser to the open the *Band Chart Display* tab.
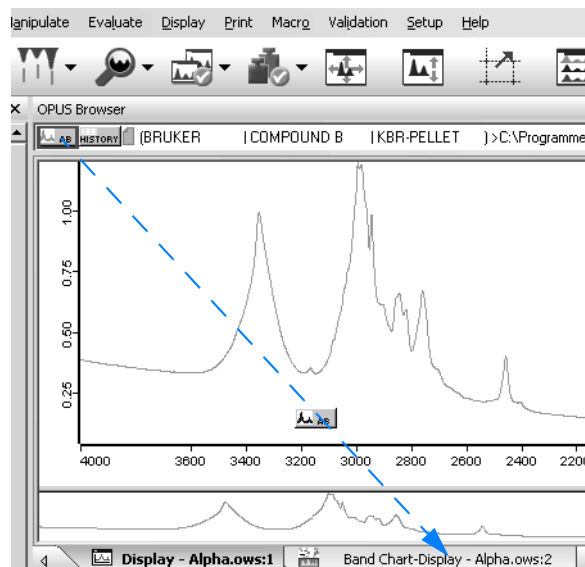
4   Drop the spectrum block into the spectrum window of the band assignment view.
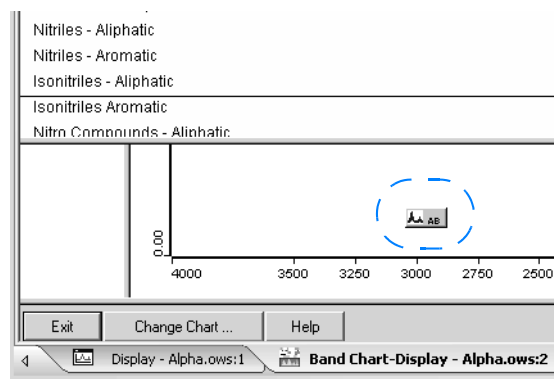
5   The spectrum is displayed in the spectrum window band assignment chart view. Note that only the last spectrum file dropped will be displayed in the spectrum window

6   A spectrum search will be performed in the band assignment chart and the entries of the upper window (A in figure 184) will be sorted according to the result of this particular search. **This means that those functional groups which spectra come very close to the spectrum displayed in the spectrum window (C in figure 184) are shown at the lowest end of the list.** Thus, you can quickly get an overview about the functional groups in the substance which forms the basis for the spectrum. Now, the browser includes the ⌗⌗⌗SEARCH data block.

7   If you right click on the spectrum window (C in figure 184), a menu pops up and provides the most important functions required to edit the spectrum display, e.g. *Zoom* and *Scale*. Depending on the spectrum range selected the chart in the upper window (A in figure 184) changes accordingly. This allows to quickly check whether the band positions in the spectrum and the chart are conform with each other.

8   If you double click on the functional group name, you can have the molecular structure displayed in the structure window (B in figure 184). The functional group name will be highlighted in light gray in the upper window. Double click again on the name to undo the selection.

To select a different band assignment chart...

1   ...click on the *Change Chart* button.

2   Select a different band assignment chart from the dialog that pops up. The information provided by the band assignment chart are stored in the OPUS library format. Therefore, it is practically possible to display OPUS libraries in the band assignment chart view, which is, however, not very useful.

3.8 Display Menu

The commands in this menu allow to modify the display of the current spectrum window. You can zoom in certain areas of the spectrum window and restore the original display size.

The availability of the commands substantially depends on the steps performed. For example, the *Forward* and *Back* commands are only enabled if you have zoomed in the current display before.
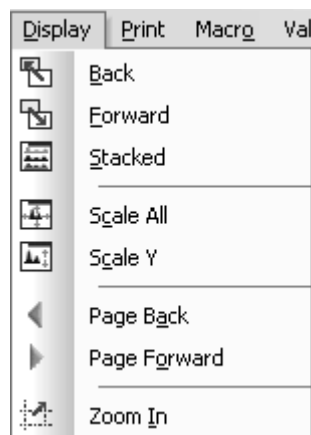
Figure 185: Display menu

3.8.1 Back /Forward

Definition	The *Back* command allows to restore the original display size of the spectrum displayed in the spectrum window, if you have first zoomed in a particular spectrum range.
	The *Forward* command displays the zoomed-in area again.
Principle	• Load a spectrum file. • Right click into the spectrum and select the *Zoom In* command from the pop-up menu. • Select a particular spectrum range. For detailed information see chapter 1.13.1. • The spectrum range selected is displayed in enlarged format. • Select the *Back* command to reduce the spectrum range to the original display size. • The *Forward* command would enlarge the spectrum range again.

3.8.2 Stacked

Definition	If more than one spectrum have been loaded into the same spectrum window, you have the option of a stacked display. In this case the spectra will not overlap. **The display in the overview window is, however, not affected by this command.**
Principle	Load several spectrum files, one after the other and select the *Stacked* command. The spectra are displayed as follows:
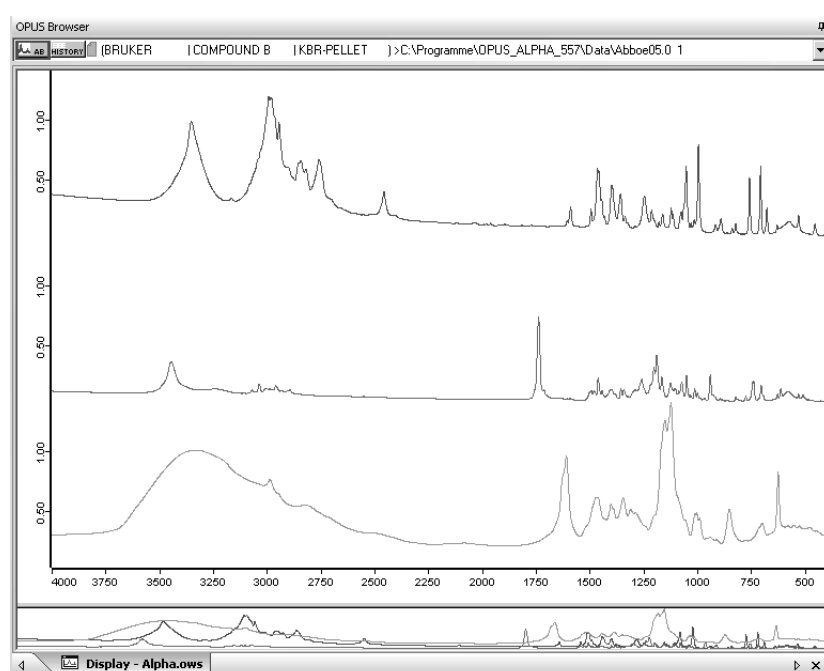
Figure 186: Spectra in stacked display mode

Note: The ordinate will automatically be duplicated when displaying several spectra in stacked mode.

To display separate axes for each spectrum...

1   ...right click into the spectrum window
2   Selecting the *Properties* command from the pop-up menu.
3   Activate the corresponding check box on the *Axes* tab.

Figure 187 shows two spectra with separate axes for each spectrum.
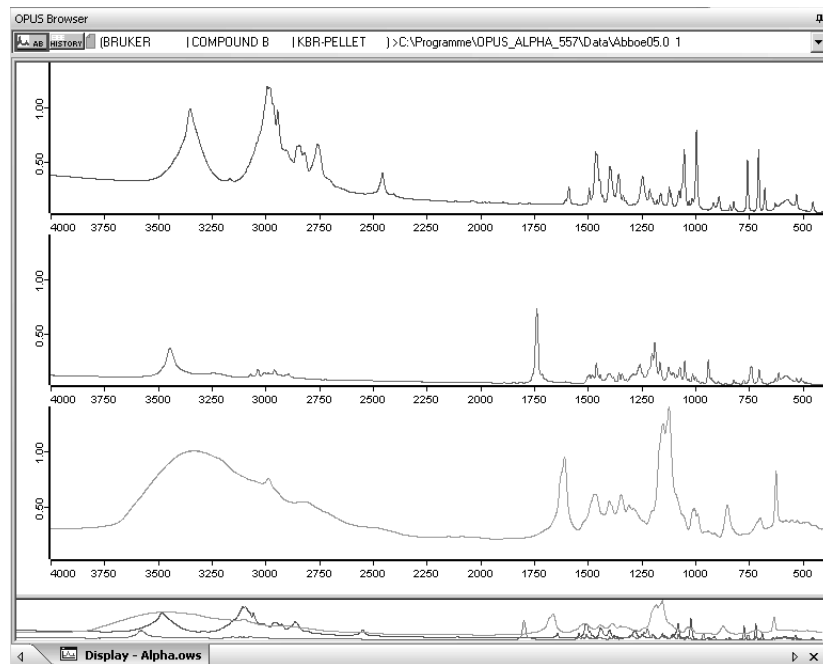
Figure 187: Spectra display with separate axes

> **Note: If you zoom in a particular spectrum range displayed in stacked mode, all the other spectra displayed in the spectrum window will automatically be affected. To undo the stacked display, click on the *Stacked* command again.**

3.8.3   Scale All ⊞/Scale Y ⊞

Definition	The *Scale All* command allows to fit a spectrum to the size of the spectrum window. To scale the ordinate only, select the *Scale Y* command.
Principle	Load the spectrum file and select the *Scale All* or *Scale Y* command.

3.8.4   Page Back ◀/Page Forward ◀

Definition	If you have selected only a particular spectrum range in the spectrum window, this range will be displayed on a white background in the overview window, while the rest appears on a gray background. The spectrum range selected can be moved along the frequency axis using the *Page Forward* and *Page Backward* commands. In this case you can browse a spectrum while keeping the displayed frequency range the same.
Principle	• Load the spectrum file. • Right click into the spectrum and select the *Zoom In* command from the pop-up menu. • Select a particular spectrum range. For detailed information see chapter 1.13.1. • The spectrum range selected is displayed in the overview window on a white background. • Select the *Page Back* or *Page Forward* command.

The display in the overview window will be as follows:
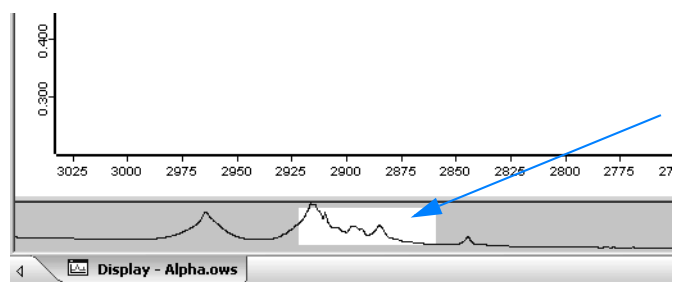
Figure 188: Particular spectrum range displayed in overview window

3.8.5   Zoom In

Definition	The *Zoom* command allows to enlarge particular spectral ranges. **See also the *Zoom in* command from the pop-up menu in chapter 1.13.1.**
Principle	• Load the spectrum file. • Select the *Zoom In* command. • A cross-hair cursor is displayed. • Use the left mouse button to draw a frame around the range you would like to enlarge. • Click on the mouse button again. The cross-hair cursor disappears and you can reposition the frame. • Left click again. The area marked by the frame will be resized to the spectrum window. • The crosshair can be removed by a right click into the spectrum window.

3.9   Print Menu

The printing functions in the *Print* menu allow to print spectra, create new printing templates or layouts, and load existing layouts.
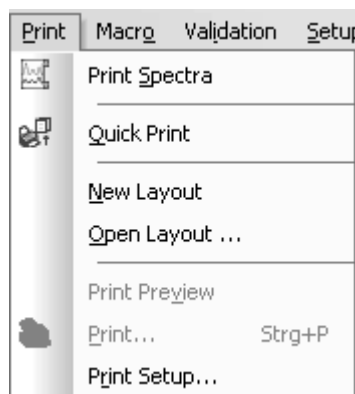
Figure 189: Print menu

The OPUS Mentor software package contains the following default plot layouts.

Plot layout	Layout for...
CORRELCHART.PLE	Band assignment chart
DEFAULT.PLE	Spectrum window

Plot layout	Layout for...
EVALRESULTS.PLE	Evaluation results
LIBRARY.PLE	Library
QCOMPRESULT.PLE	Quick compare results
REPORT.PLE	Reports
SEARCHRESULTS.PLE	Search report

Plot layouts have the extension *.*PLE* and can consist of different frames, e.g. spectrum or text frames, as well as of tables. For detailed information on the plot layout elements refer to chapter 3.9.3.

3.9.1   Print Spectra

Definition	The *Print Spectra* command allows to print spectra from OPUS.
Principle	• Load the spectrum file and select the *Print Spectra* command. • A dialog opens which automatically contains the name of the spectrum file in the *File(s) to print selected frame* selection field. • Select a plot layout. • Define the frequency limits on the *Frequency Range* tab. • Define the output format on the *Options* tab. • Click on the *Print* button. **Note: Before printing spectra, make sure that you have installed a default printer first.**

The different tabs of the *Print Spectra* dialog are described in the following.

Select Files
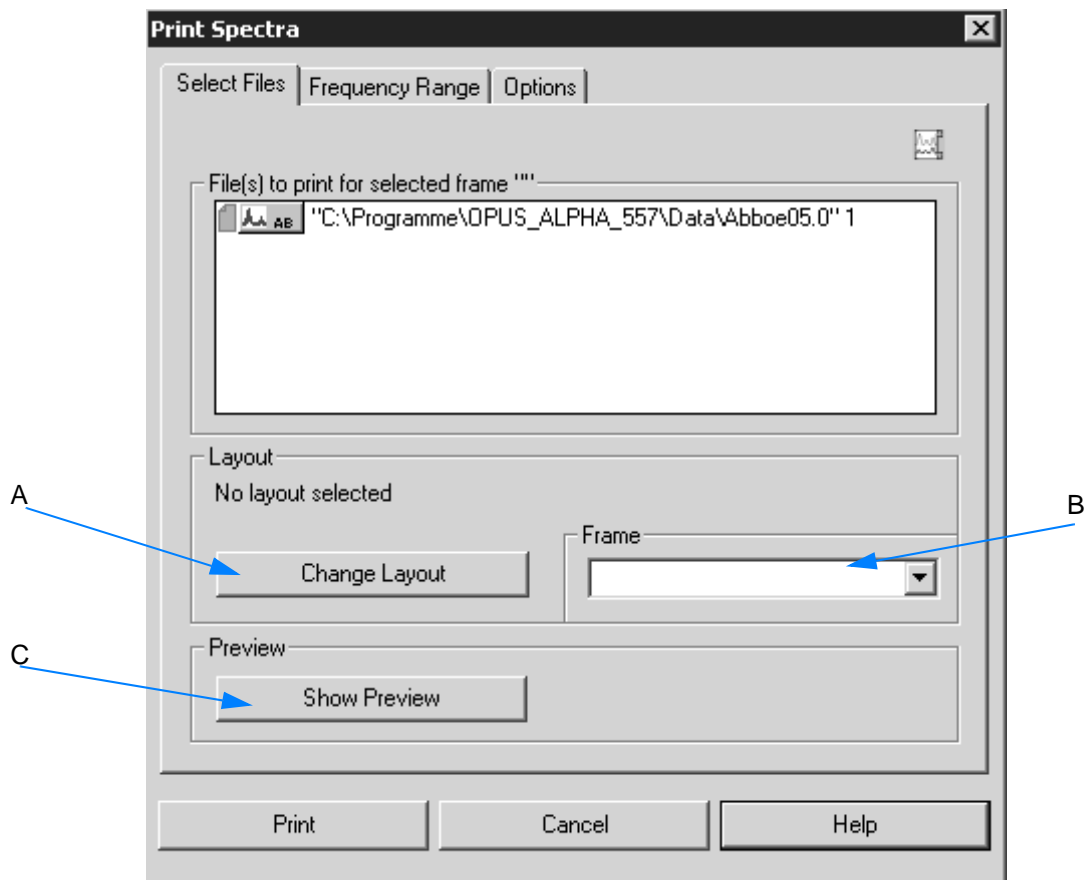
Figure 190: Print Spectra - Select Files

Selecting plot layout

1 Click on the Change Layout button (A in figure 190).

2 The *Select Print Layout* dialog opens.

3 Select a plot layout. **Plot layouts are stored in <OPUS> and have the extension .*PLE.** If you have selected a plot layout, the name and path of this layout will be displayed. **By default, the plot layout last selected for printing is displayed.**
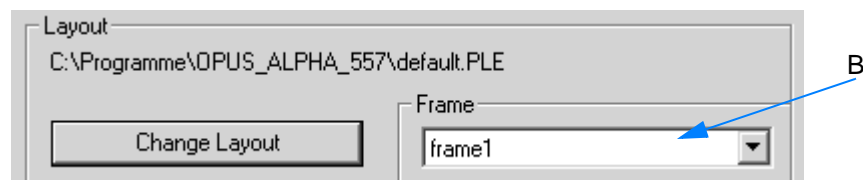
4 You can select the frames included in a particular plot layout from the *Frame* drop-down list. Each data block of a spectrum file can have a special frame.

Example: If you select *frame 1* and the *AB* data block is displayed in the *File(s) to print for selected frame* selection field, the *AB* data block will be printed in frame 1. This will also be indicated in the selection field header.

To know what the different frame descriptions included in a plot layout mean click on the *Edit Layout* button in the *Select Print Layout* dialog.
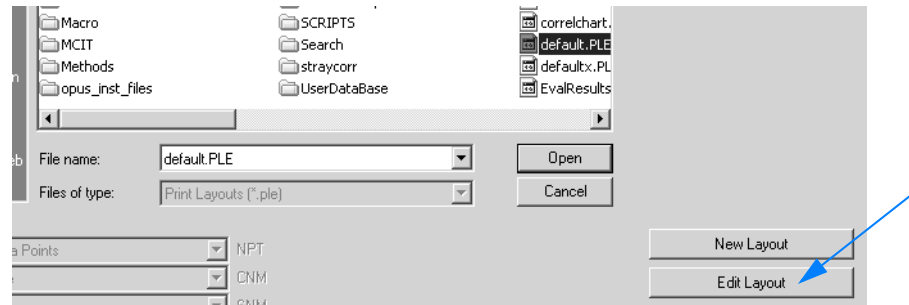
The plot layout interface opens. The frame definition is indicated in the *Item* column. For further details on this subject refer to chapter 3.9.3.2.
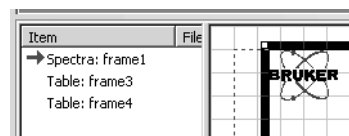
Show Preview

To display a preview of the plot click on the *Show Preview* (C in figure 190) button. If the plot consists of several pages, you can select between a single and two-page display and scroll through the single pages. Additionally, you can zoom in or out the spectrum previewed.
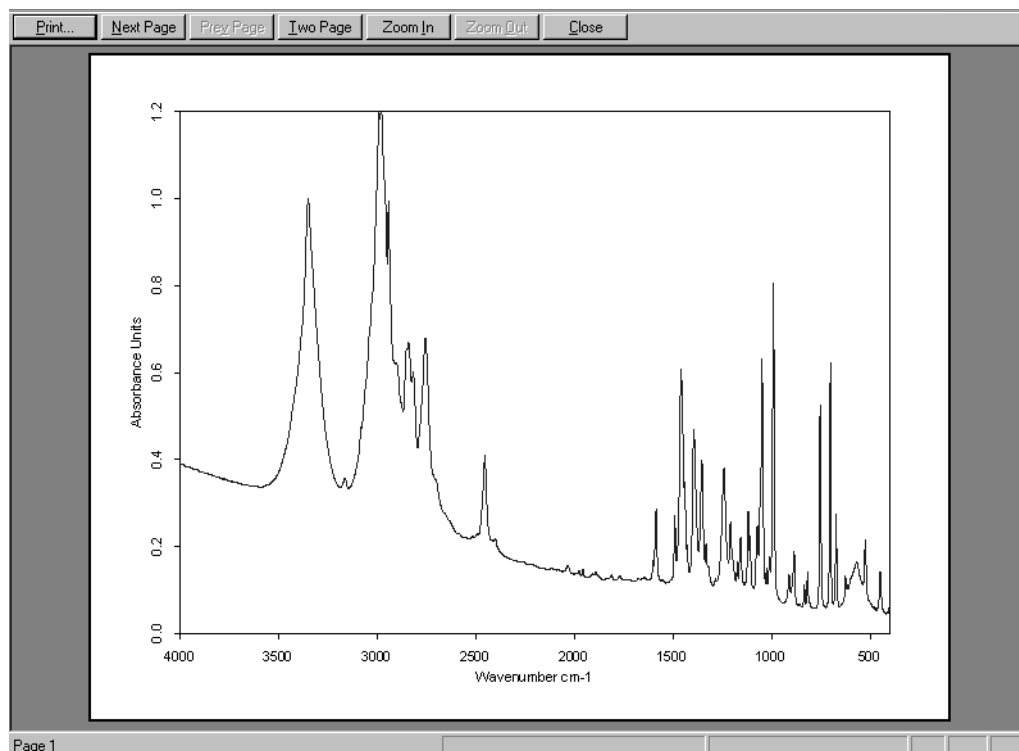
Figure 191: Print Preview

Frequency Range
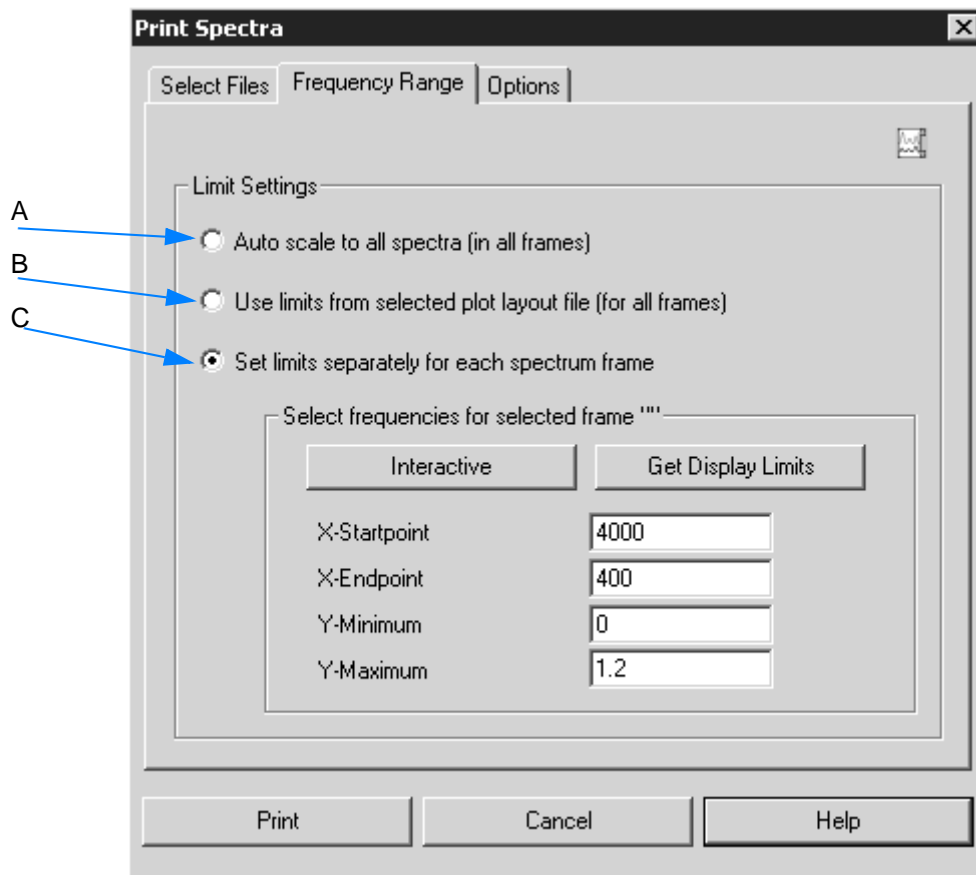
Figure 192: Print Spectra - Frequency Range

A If you activate this option button, the axis of all spectra in all frames will be set to their maximum size.

B If you activate this option button, the frequency limits of the plot layout selected before will be used.

C As soon as you activate this option button, the *Select frequencies for...* group field will be enabled. Either type the limit values manually or define them interactively (see chapter 1.14).

If you click on the *Get Display Limits* button, the current limits displayed in the spectrum window are automatically set in the appropriate entry field.

Options
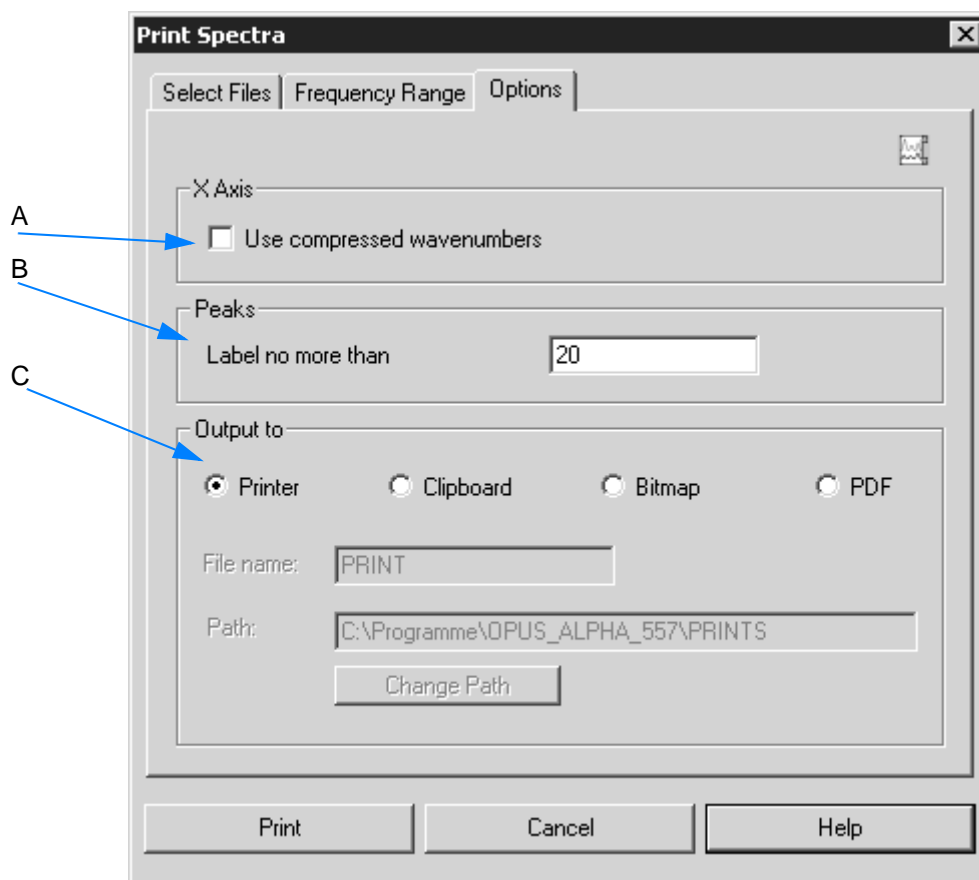
Figure 193: Print Spectra - Frequency Range

A If you activate this check box, the compressed wavenumbers are plotted, i.e. the wavenumbers above 2000cm^{-1} will be compressed by a factor of 2.

B Define the maximum number of peaks which are to be labelled.

C Define the output format. The printout can both be sent to the printer or the clipboard. It is also possible to create a bitmap or a PDF file.

If you activate the *Bitmap* or *PDF* option button, the *File name* and *Path* entry fields are enabled. To save the printing define the file name and path or edit the path by means of the *Change Path* button.

3.9.2   Quick Print

Definition	The *Quick Print* command allows to plot the contents of an OPUS view without specifying a template. An appropriate default template for the currently displayed view will be used.
Principle	Quick Print means that a printout is generated which shows the OPUS window as displayed on the screen. If only part of the spectrum is displayed, only this part will be printed including possible labels and annotations.

3.9.3   New Layout

Definition	The *New Layout* command allows to create new layout templates using the plot layout editor (PLE).
Principle	The plot layout editor consists of a separate view. This view opens when clicking on the *New Layout* command.

To create a new layout template...

1   ...select the *New Layout* command.
2   The PLE view opens.
3   Create the template by means of the icons and pop-up menus.
4   Store the template by clicking on the *Save as* command in the *File* menu on the PLE view. **Template layouts have the file extension **.PLE.***

The PLE view is described in the following.
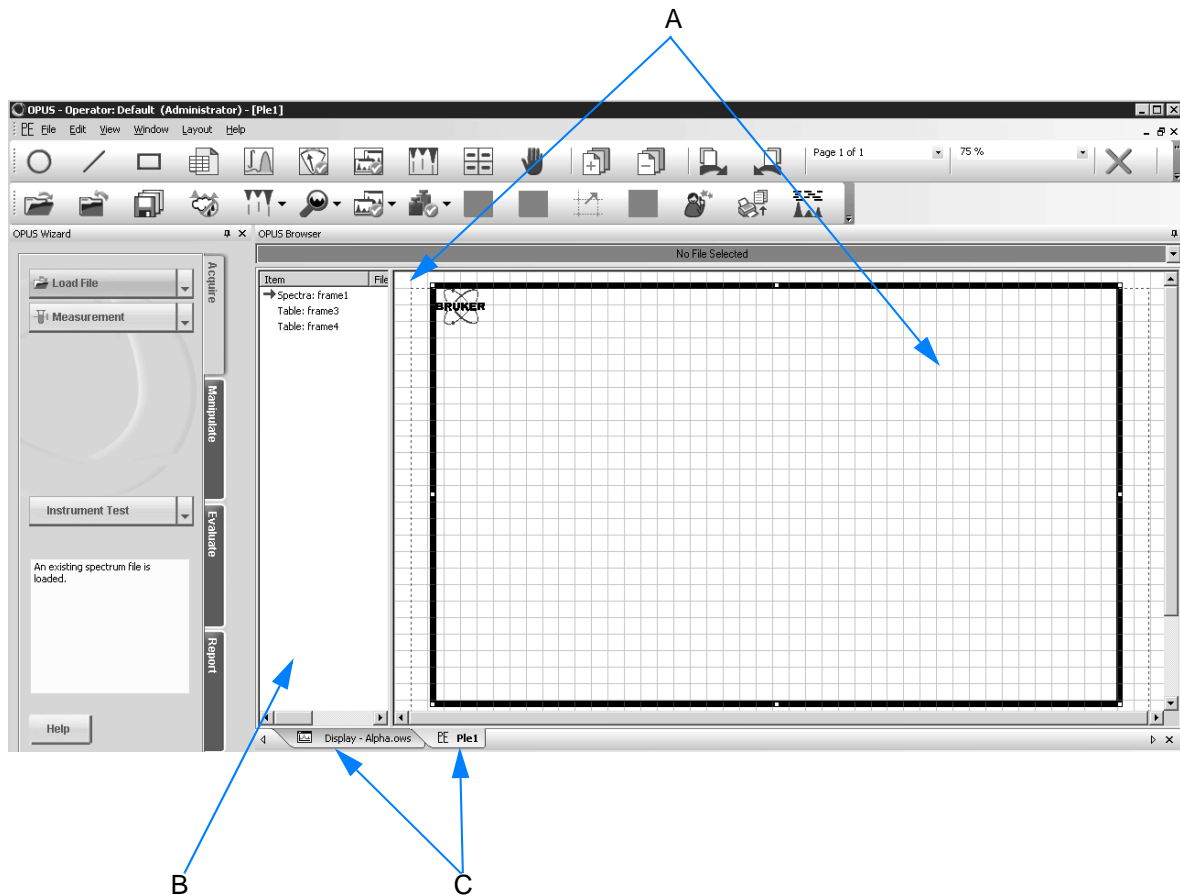
Figure 194: PLE view

    A The PLE drawing area consists of a black grid and a red broken-line frame. This frame represents the available print area of the printer.

    B Directly to the left is the PLE item window (C) which shows all items displayed on the PLE drawing area.

    C To switch between PLE view and the OPUS spectrum window use the *Display* or *PLE* tab.

3.9.3.1 PLE icons

The PLE icons required to create layout templates are provided on a separate toolbar, and are listed in the following table.

Icon	Definition
⬭	Drawing a circle or ellipse
╱	Drawing a line or an arrow

	Drawing a frame
	Drawing a table frame
	Drawing an integration report frame; the report frame will automatically be linked to the spectrum frame (*frame1*)
	Drawing a QUANT report frame; the report frame will automatically be linked to the spectrum frame (*frame1*)
	Drawing a quick compare report frame; the report frame will automatically be linked to the spectrum frame (*frame1*)
	Drawing a peak report frame; the report frame will automatically be linked to the spectrum frame (*frame1*).
	Drawing a standard parameter table; the table frame will automatically be linked to the spectrum frame (*frame1*)
	Selecting and moving items
	Adding page (in case of multi-page templates)
	Removing page (in case of multi-page templates)
	Selecting next page (in case of multi-page templates)
	Selecting previous page (in case of multi-page templates)
Seite 1 von 1	Selecting active page (in case of multi-page templates)
75 %	Zooming in or out screen views. The zoom factor does not affect the actual template size. The drop-down list also includes the *Fit whole page* and *Fit page width* options.
	Deleting items
	Deleting item contents
	Opening *PLE page properties* dialog (see chapter 3.9.3.4)
	Opening *Spectral Frame properties* dialog (see chapter 3.9.3.5)
	Anchoring object frame or undo anchoring

3.9.3.2 Items

The *Item* column (B in figure 194) shows all items displayed on the drawing area.

Frames will be referred to by the type of data included (table, spectrum etc.). The active frame is indicated by a red arrow in the item window and marked by a thick line on the PLE drawing area.
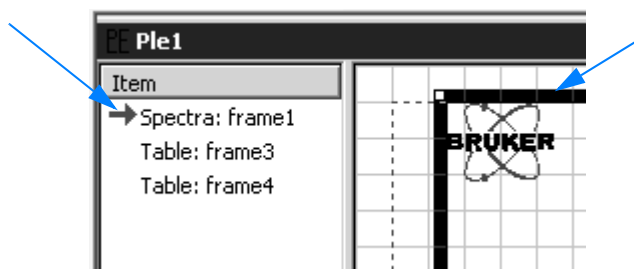
Figure 195: Active frame display

Each new frame created is named *frame_x*, with *x* being automatically incremented. To activate a particular frame you have to select it. Left click either on the frame displayed on the drawing area, or on the name of the frame indicated in the *Item* column.

3.9.3.3 Pop-up menu

If you right click on a frame, the PLE pop-up menu opens. This menu allows to individually configure the frame.
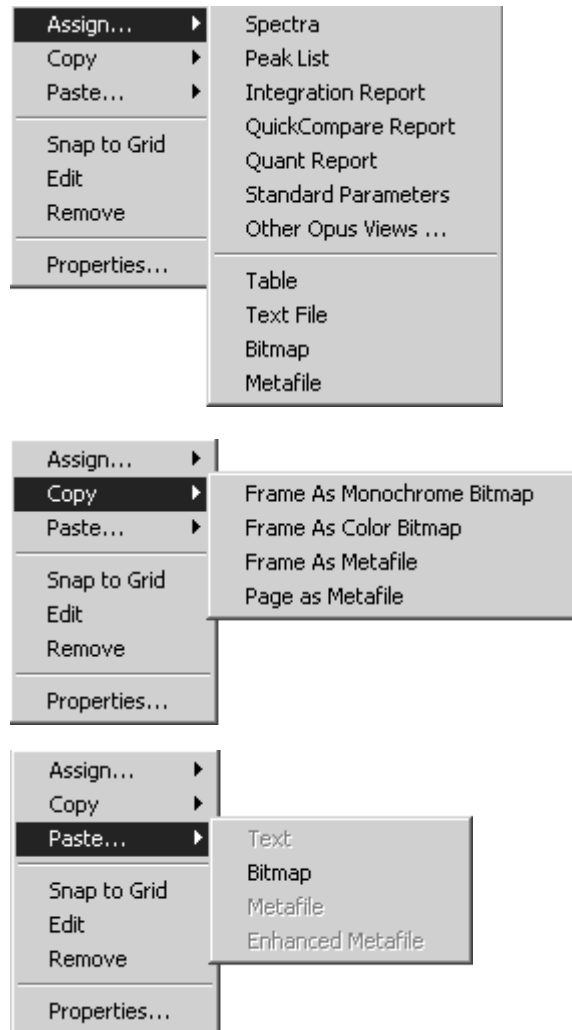
Figure 196: PLE pop-up menu

To change the contents of a frame use the *Assign* command. You can assign spectra, peak lists, standard parameters and other OPUS views as well as reports to a frame.

The *Copy* command duplicates the content of a frame as monochrome bitmap, color bitmap or meta file. The content of a page can be copied as metafile.

By means of the *Paste* command you can insert text, a bitmap, meta file or text from the clipboard into the active frame.

The *Remove* command deletes the frame from the drawing area, while the *Snap to Grid* command aligns this frame exactly on the closest grid lines.

The *Edit* command allows to manipulate the frame contents. This command is only available for text and table frames.

If you select the ***Properties*** command, the *Properties* dialog of the selected frame opens.

3.9.3.4 Drawing area

As the available drawing area (A in figure 194 on page 204) depends on the printer setup you first have to configure the particular printer settings.

1   Select the *Print Setup* command from the *File* menu in the PLE view.

2   Click on the *Properties* button and set the appropriate paper size and format.

3   Confirm the settings by clicking on the *OK* button.

The PLE drawing area visually represents the plot view of the current template, containing all the frames. Each frame can be scaled and positioned individually. Below the drawing area two co-ordinates are displayed.
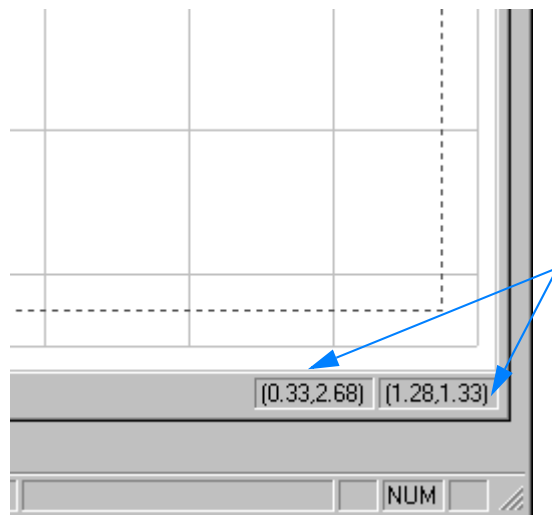
Figure 197: Co-ordinates of the drawing area

The left co-ordinate indicates the exact position of the active frame on the drawing area, the right indicates the frame size. Even if you resize the frame the current size is always shown in the corresponding co-ordinate display.

To resize the drawing area...

1   ...right click somewhere on the drawing area.
2   The *Ple Page* dialog opens.
3   Use the different tabs of this dialog to define general settings for the drawing area.
4   To confirm the settings click on the *OK* button.

The different tabs of the *Ple Page* dialog are described in the following.

Page
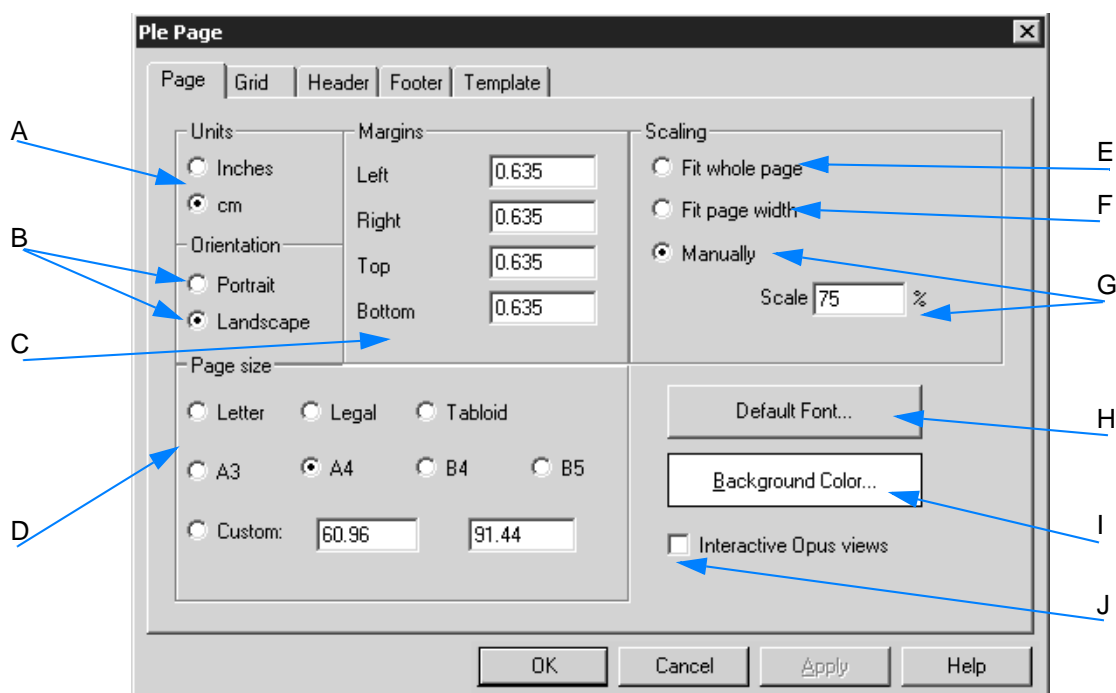
Figure 198: Ple Page - Page tab

A Specify the unit that you want to work with (inches or centimeters).

B You can print either in landscape or portrait.

C Define the maximum print area. Each printer has a particular margin used for paper feed, and which will not be printed on. These default settings are suitable for all common printers and have to be rarely adjusted. **The maximum print area is represented by a dotted red line on the PLE document.**

D Define the paper size. The corresponding unit has been defined by (A).

E Check this option button if the drawing area is to be enlarged up to the size of the whole page.

F Check this option button if the drawing area is to be enlarged up to the page width.

G If you check this option button, the entry field will be enabled. Enter the scale factor manually. The scale factor required to view the PLE pages is indicated in per cent. Most monitors are not large enough to allow viewing the entire page at 100% scale. **In case of landscape orientation it is advisable to use a scale factor of 75%, in case of portrait orientation a scale factor of 50%.**

H Specify the default font to be used when creating a frame within a document. If a frame includes data, the font can be changed no matter what kind of default setting you use.

I Define the background color of the view.

J If you activate this check box, you can assign any type of OPUS view to a frame.

Draw a frame on the PLE drawing area and right click onto the frame. Select the *Assign → OPUS View* command from the pop-up menu. The drop-down list includes all OPUS views available. If you have selected a structure view, you can drag & drop a structure data block ( ) into the frame. To save the PLE page as template it is advisable to remove the data block again, and the frame will only include the view type assigned to.

Grid
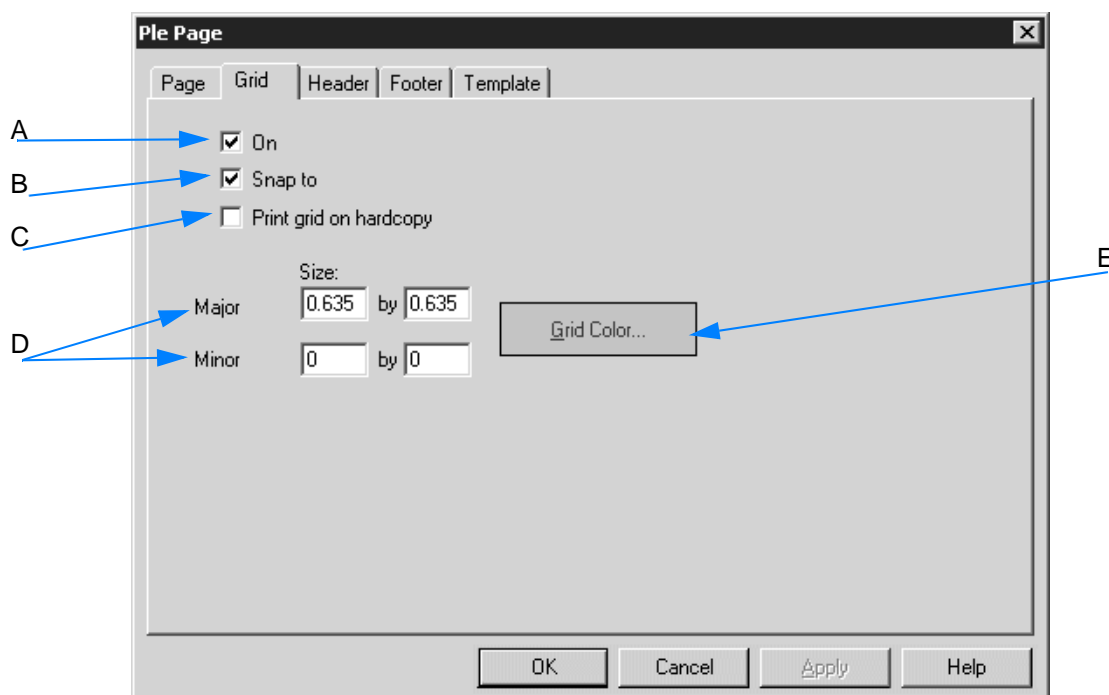
Figure 199: Ple Page - Grid tab

A If you activate the check box, the grid will be visible. The grid can be useful to align objects on the drawing area.

B If you activate the check box, new objects created are automatically positioned and sized to line up with the closest major grid lines.

C Usually, the grid is only displayed on the screen to simplify object alignment. Activate the check box if you want to have the grid printed on paper.

D The *Major* and *Minor* settings define the grid size in the unit specified on the *Page* tab. Figure 199 exemplifies a grid size of 0.635 x 0.635 inch. The grid can be further divided by filling in the *Minor* entry fields.

E If you click on the *Grid Color* button, a color palette opens. Select or define the color for the grid.

Header

The header and footer are printed on every page. The *Header* and *Footer* tabs are identical, therefore only the *Header* tab will be described in the following.
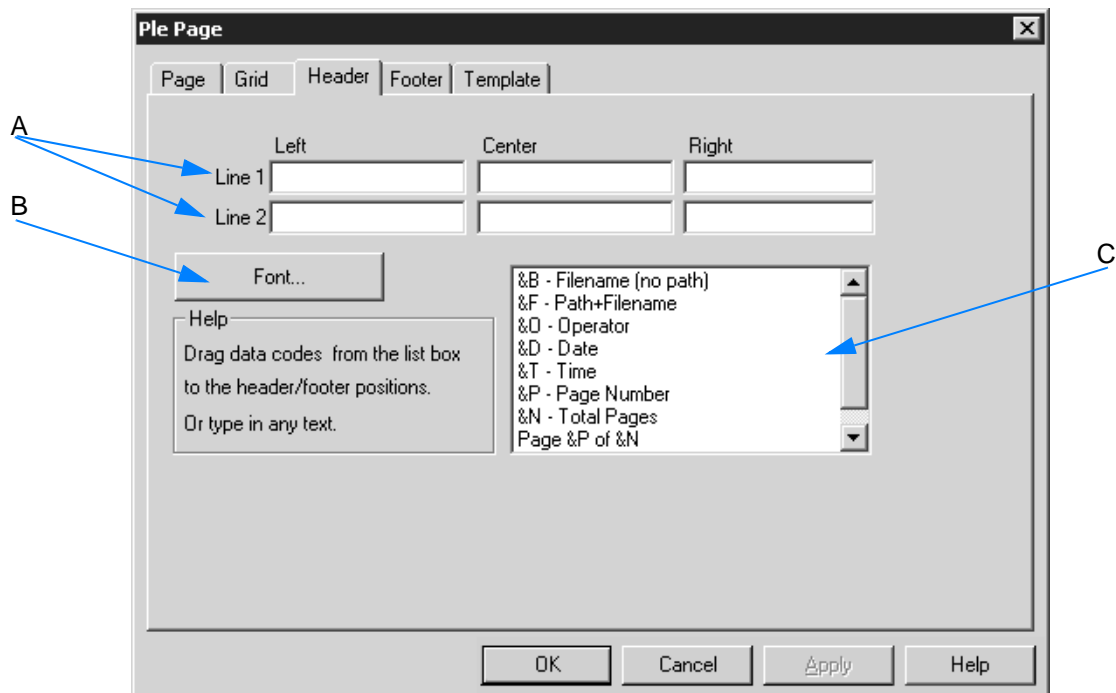
Figure 200: Ple Page - Header tab

A The header (or footer) can consist of up to 6 fields (2 rows on the left, middle and right). The entries in the fields consist of meta strings (also see chapter 3.9.3.6). You can either enter these meta strings manually or drag & drop them using the list box (C). It is also possible to enter plain text for the header or footer.

B Click on the *Font* button to define the header font.

C The list box includes special meta strings. The editor automatically converts these meta strings into readable text in the preview. You can drag & drop these commands from the list to the particular entry field which you want to have the information printed in.

Template
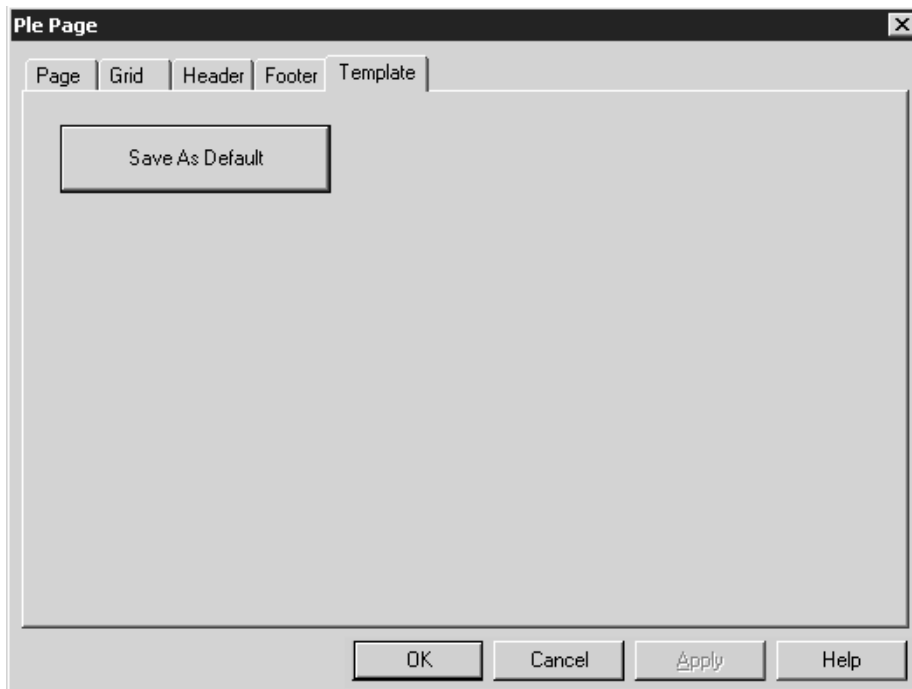
Figure 201: Ple Page - Template tab

You can save a particular template as default. When creating new PLE documents the settings of this particular template will be used.

> **Note: The default template automatically has the extension *default.ple* and is located in the same directory as the OPUS program.**

The *Save As* command in the *File* menu allows to save templates, using any file name and directory. To load these templates use the *Load File* command from the *File* menu.

3.9.3.5 Adding spectrum and modifying spectrum frame

There are two possibilities to load a spectrum to the drawing area:

1   Drag & drop the spectrum from the browser directly into the spectrum frame on the drawing area. Load the spectrum file from within the PLE view. The spectrum window is displayed again. Drag the spectrum data block (AB or TR) from the browser to the

 PLE tab (PE **Ple1**). Wait until the PLE view opens by pressing the left mouse button. Drop the spectrum block into the spectrum frame.

2   Draw a frame by using the ▢ icon and assign the spectrum to this frame. Right click on the frame and select the *Assign → Spectra* command from the pop-up menu. Select the particular spectrum from the dialog that opens. The spectrum is shown within the frame.
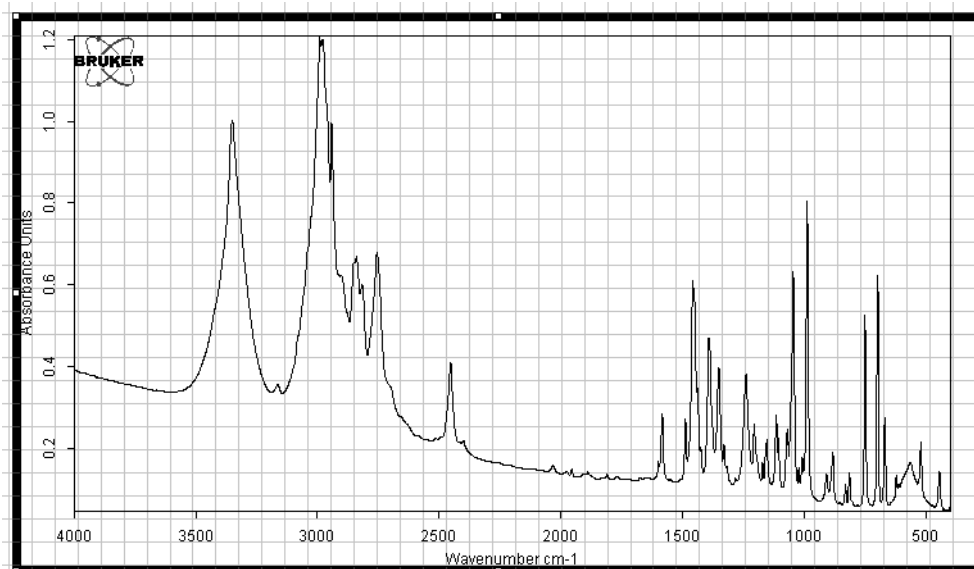
Figure 202: Frame with spectrum

To have the standard spectrum parameters displayed...

1   ...click on the ⊞ icon in the toolbar.

2   Press the left mouse button and draw a frame onto the drawing area. This frame includes a table which consists of rows and columns, by default.

Sample Name	^SNM	Aperture Setting	^APT
Sample Form	^SFM	Beamsplitter Setting	^BMS
Operator Name	^CNM	Detector Setting	^DTC
Resolution	^RES	Source Setting	^SRC
Scantime or Scans	^SOS	Measurement Channel	^CHN
Sample Scans	^NSS	Acquisition Mode	^AQM
Start Frequency Limit for F	^LFQ	Phase Correction Mode	^PHZ
End Frequency Limit for Fi	^HFQ	Apodization Function	^APF

Figure 203: Table frame including standard spectrum parameters

3   If you want to change these default name settings, right click on the table and select the *Edit* command from the pop-up menu. This allows to directly get into the table cell to change the text.

4   If you want to change the table size, right click on the table frame and select the *Properties* command from the pop-up menu. The *Table Properties* dialog is displayed. For detailed information refer to chapter 3.9.3.7.

To modify the spectrum frame...

1   ...right click into the spectrum frame.

2   Select the *Properties* command from the pop-up menu.

3   The *Spectral Frame Properties* dialog opens.

4   Use the different tabs of this dialog to define general settings for the spectrum frame.

5   To confirm the settings click on the *OK* button.

The different tabs of the *Spectral Frame Properties* dialog are described in the following.

Item
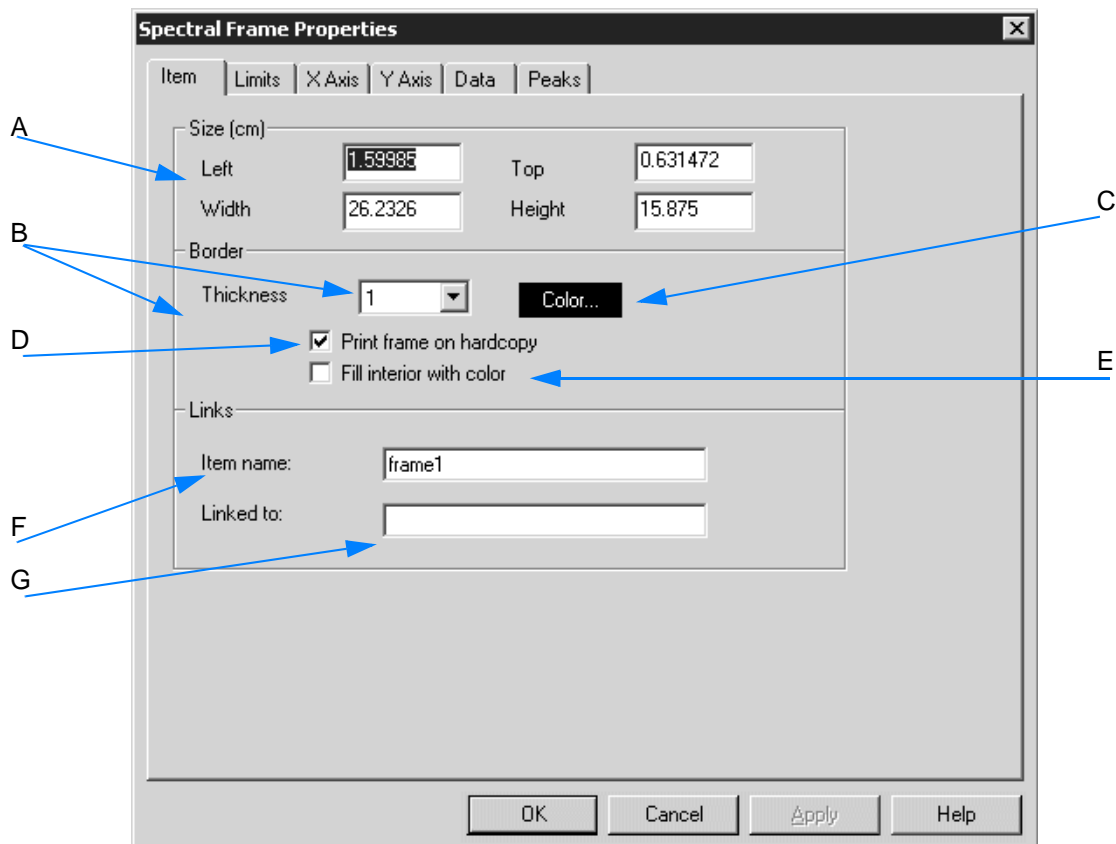
Figure 204: Spectral Frame Properties - Item

A   To change the size and position of the frame on the drawing area use these entry fields. The unit (cm or inch) has been specified by the *PLE Page* dialog on the *Page* tab (see chapter 3.9.3.4).

B   The line thickness used for the frame is indicated in pixels in the drop-down list.

C   Using this button allows to define the frame contour color. If you click on the *Color* button, a color palette opens. Select or define the color desired.

D   Normally, the frame contour is not printed. If you activate this check box, the contour will also be printed on hard copy.

E   If you activate the check box, the frame will be filled by the color specified in (C).

F   You can assign a name to any item. This is advisable in case of complex layout templates as a name simplifies the identification of the object. You can use this name to link tables and text frames to spectrum frames.

G   This entry field includes the name of a particular link. **This option is only reasonable in case of tables, report frames and texts.**

If you want to add e.g. data from a particular spectrum frame to a table, enter the name of the spectrum frame into the *Linked To* entry field. This entry has to be adjusted as soon as the name of the respective spectrum name has been changed by the operator. Otherwise, the link between the different frames will be lost.

Limits
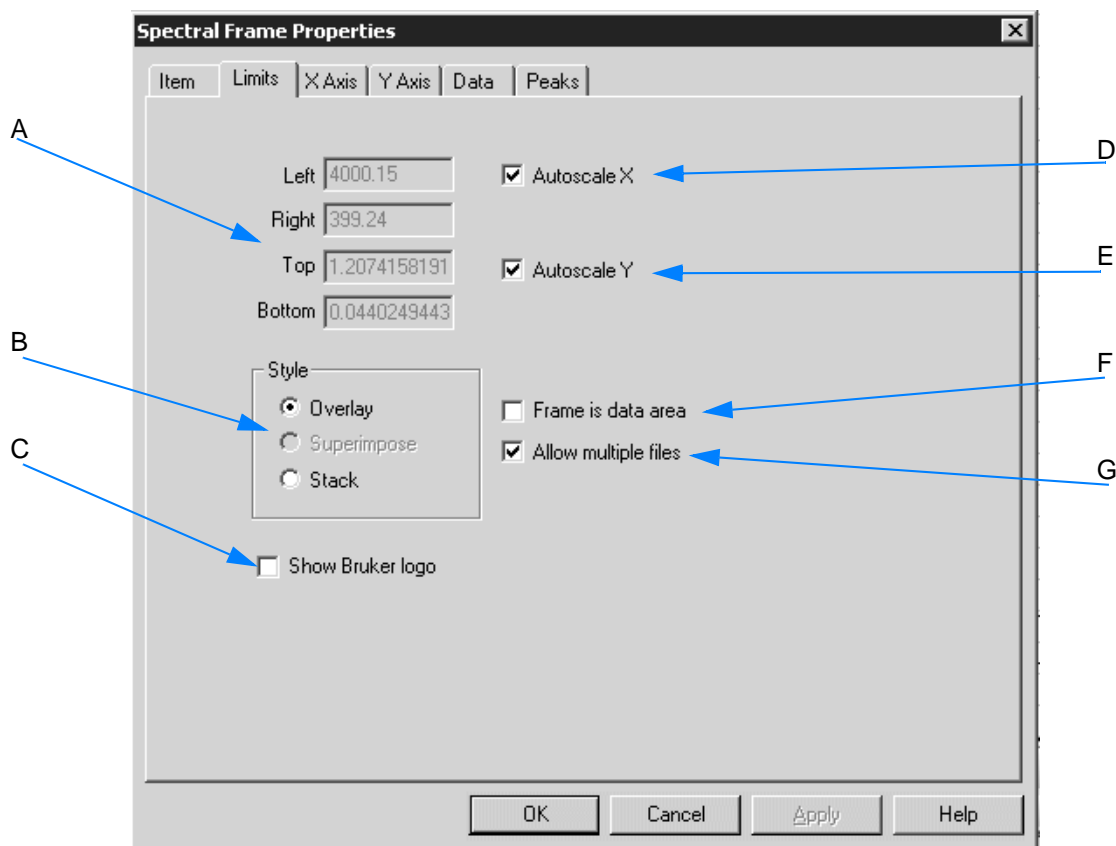
Figure 205: Spectral Frame Properties - Limits

A   The entry fields allow to define the frame limits. The unit of the values entered has been specified in the *PLE Page* dialog on the *Page* tab (see chapter 3.9.3.4).

B   The style type selected determines the data depiction within the frame. You can have the spectra displayed in overlaid or stacked mode.

C   Activate the check box if you want to have the logo displayed within the spectrum frame.

D   If you activate the check box, the spectra x axis will be autoscaled within the frame.

E   If you activate the check box, the y axis of the spectra will be autoscaled within the frame.

F   The frame displayed on the drawing area can either include the entire spectrum (with axes and annotations), or can be used as outer line of the spectrum itself. If you activate the *Frame is Data Area* check box, the axes and annotations will be drawn outside the frame.

G   If you do not activate the check box, only one spectrum can be displayed within the frame.

Axes

The *X Axis* and *Y Axis* tabs are identical except for the *Rotate Numbers* check box on the *Y Axis* tab. This option allows to rotate the y axis annotations by 90°. The *Show axis for stacked spectra* and *Compressed Wavenumbers* check boxes are only available for the x axis.
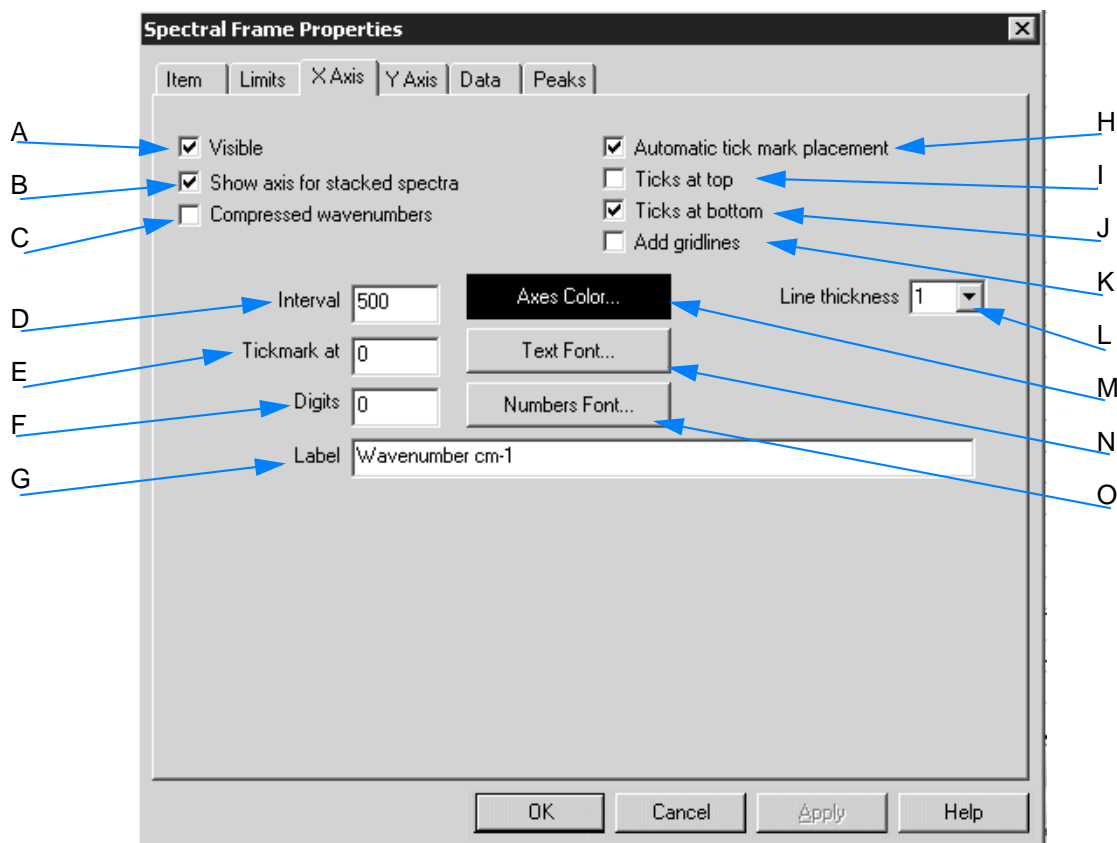
Figure 206: Spectral Frame Properties - x Axis tab

A Activate the check box if the axes, tick marks and labels have to be displayed.

B Activate the check box if each spectrum has to be displayed with a separate x axis. Otherwise, one common x axis will be used for all spectra loaded.

C If you activate the check box, wavenumbers above 2000cm^{-1} will be displayed using a smaller linear scale.

D If you have not activated the *Automatic Tick Mark Placement* check box (H), you can specify the interval between two tick marks.

E In the *Tickmark at* entry field you determine the position of a tick mark, provided you have not activated the *Automatic tick mark placement* check box (H).

F Specify the number of digits used for the numeric tick mark labels, provided you have not activated the *Automatic tick mark placement* check box (H).

G The axes are labelled according to the spectrum file loaded by the editor. The axis label can be changed. In this case enter text into the entry field.

H The editor can automatically sub-divide axes if you activate the check box.

I If you activate the check box, the tick marks will be displayed on top of the frame.

J If you activate the check box, the tick marks will be displayed at the bottom of the frame.

K Activate this check box if you want to have the grid lines displayed on the frame.

L The drop-down list allows to determine the thickness of the axis lines. You can also enter the thickness manually.

M Using this button allows to define the axes color. If you click on the button, a color palette opens. Select or define the color desired.

N If you click on the button, a list box will be displayed. Use this list box to determine the font and size of the axis label.

O If you click on the button, a list box will be displayed. Use this list box to determine the font and size of the tick mark (numeric) labels.

Data
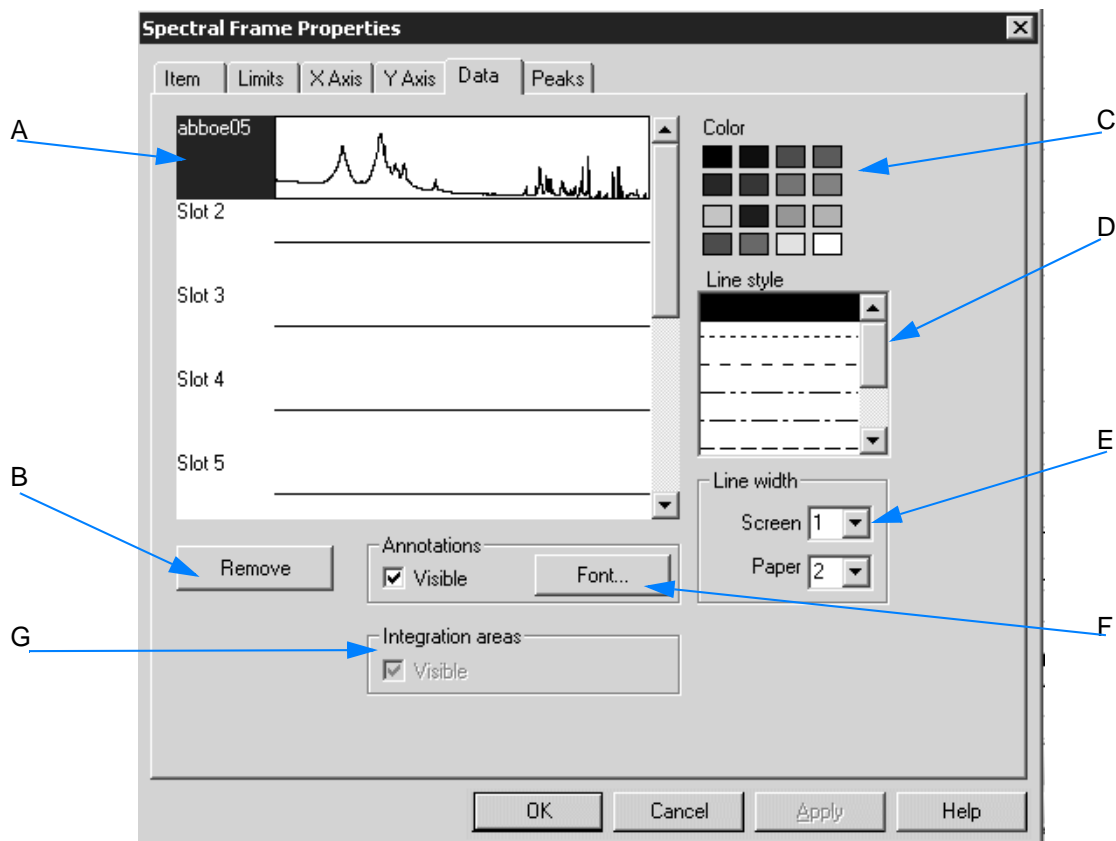
Figure 207: Spectral Frame Properties - Data

A Spectra added to a frame, are put into a slot. This slot determines the position of spectra. To change a spectrum view, you first have to select the corresponding slot of the spectrum. Then, you have to define the properties for that slot using the control elements for color, line style and line width.

B If you click on the button, the spectra data selected in (A) will be deleted from the slot.

C The color palette allows to determine the color of the spectrum displayed.

D Use the list box to determine the line style of the spectrum displayed.

E Define the line width of the spectrum displayed. Separate line widths can be specified for the screen view and printout.

F **This option is only enabled if the spectrum file contains a** **data block.** This data block can be displayed in the PLE template by activating the *Visible* check box. Use the *Font* button to determine the font for the annotations.

G **This option is only enabled if the spectrum file contains a** **data block.** This data block can be displayed in the PLE template by activating the *Visible* check box.

Peaks
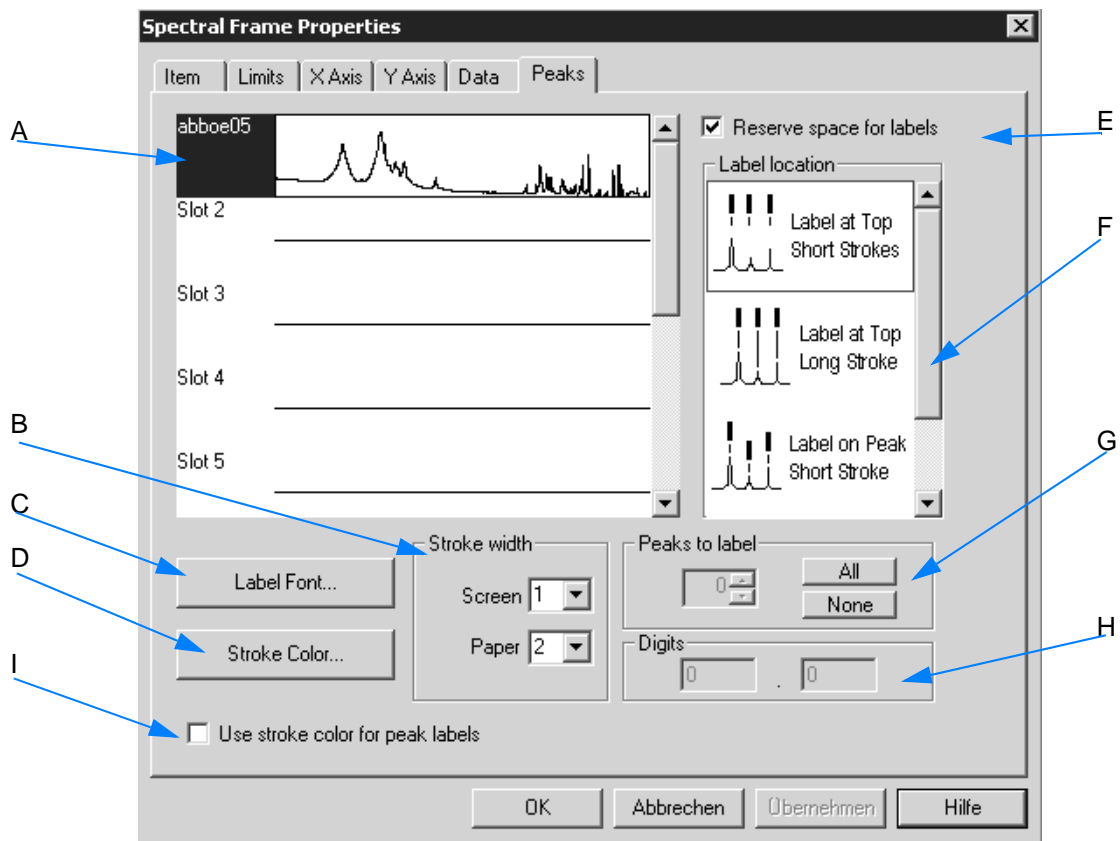
Figure 208: Spectral Frame Properties - Peaks

A   Spectra added to a frame, are put into a slot. This slot determines the position of spectra. To change a spectrum view, you first have to select the corresponding slot of the spectrum.

B   Define the stroke width of the spectrum displayed. Separate line widths can be specified for the screen view and printout.

C   Click on the button to determine the font type used for the labels.

D   Click on the button to determine the color for the label strokes.

E   If you activate the check box, extra space between the highest peak and the spectrum frame for the peak labels is provided.

F   Use the list box to select the type and position of the labels you want to assign to the peaks.

G   **This option is only enabled if the spectrum file contains a [PEAKS] data block.** Starting with the highest peak you specify the number of peaks to be labelled, using the *All* and *None* buttons.

H   **This option is only enabled if the spectrum file contains a [PEAKS] data block.** Enter the number of digits and decimals for the peak labels.

I   Activate this check box if the stroke color has to be the same as the one for the spectrum labels. This helps to get a clear display, which

is especially useful if the PLE view consists of more than one spectrum. By means of the *Stroke Color* button (D) you can define an individual stroke color for each spectrum, which will be the same for the spectrum label if you activate the check box (I).

3.9.3.6　Adding text and modifying text frame

Text can be included using text frames, i.e. either enter text manually into, or import an existing text file to a frame.

For manual text input...

1　...draw a frame by means of the ☐ icon.
2　Right click on the frame.
3　Select the *Edit* command from the pop-up menu. This will transform the frame into a text frame.
4　Now, enter text into the entry field displayed.
5　Close this entry field by left-clicking anywhere outside the field.

Note: **In case of manual text input you can also use meta strings. The meta strings used for text parameters can be directly typed into a text frame, and will be interpreted by the editor using the data from the spectrum frame linked to the text frame.**

To resize the text frame...

1　...left click into the frame and scale it up or down using the marker positions.
2　To edit text use the *Edit* command from the pop-up menu. Right click into the text frame to select this command.

To import a text file...

1　...draw a frame by means of the ☐ icon.
2　Right click on the frame.
3　Select the *Assign → Text File* command from the pop-up menu.
4　Specify the particular text file from the dialog displayed. **Note that only files with the extension *.txt* can be imported.**

To modify the text frame...

1   ...right click into the text frame.

2   Select the *Properties* command from the pop-up menu.

3   The *Spectral Frame Properties* dialog opens.

4   Use the different tabs of this dialog to define general settings for the spectrum frame.

5   To confirm the settings click on the *OK* button.

The *Text* and *Parameters* tabs of the *Text Properties* dialog are described in the following. For details on the *Item* tab refer to chapter 3.9.3.5.

Text
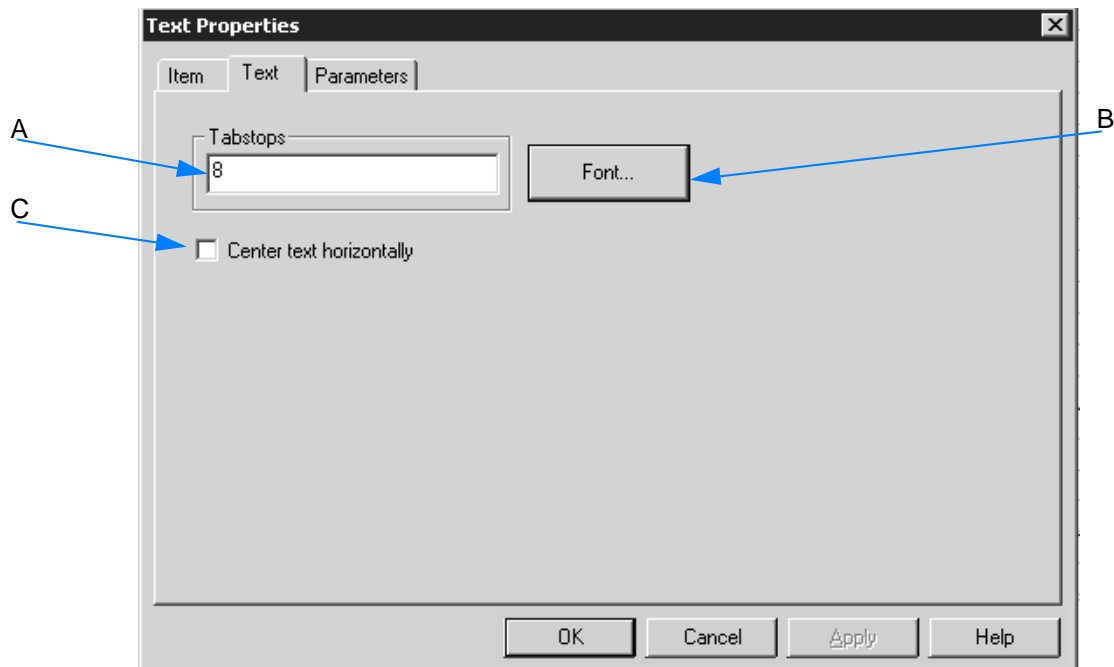
Figure 209: Text Properties - Text tab

A Defines the position of tab stops for the text in the frame. The value entered represents the distance to the next tab. Multiple positions can be used, separated by spaces, e.g. 8 12 20 40. The last tab spacing is used for subsequent tab stops, if more tabs are required.

B By means of this button you determine the font and font size of the text.

C To better align text within a frame activate the check box, as the text lines will be horizontally centered.

Parameter
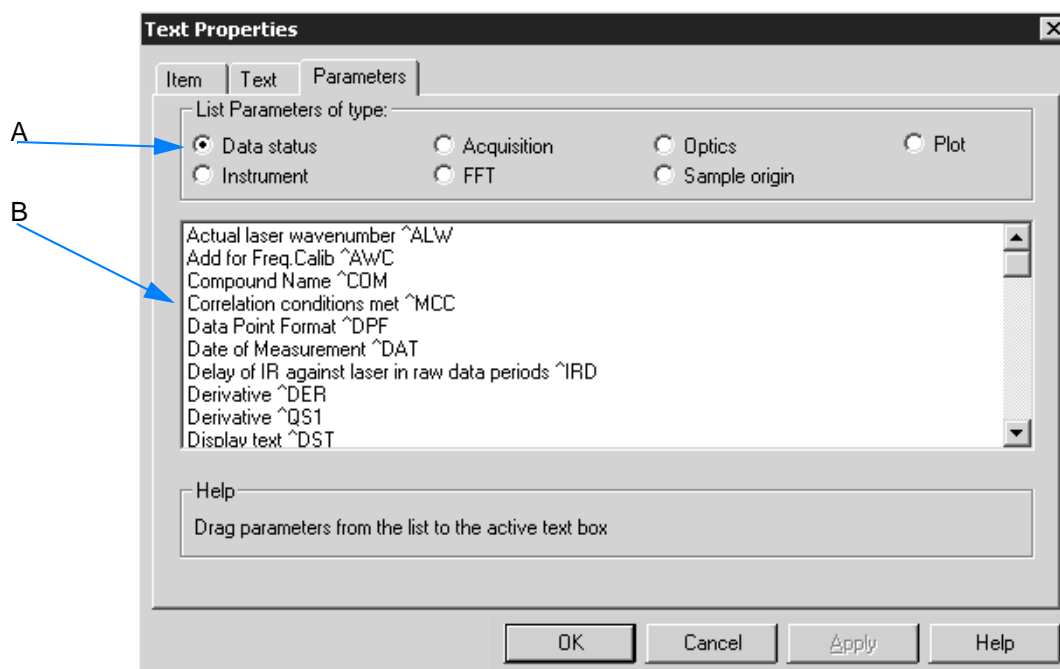
Figure 210: Text Properties - Parameters tab

A Different types of parameters are available. Select one of them.

B The entries of the list box depend on the type of parameter selected (A). To add information to a table, select an item from this list box and drag & drop it to the particular table cell.

The entries in the list box are meta strings, i.e. three-letter codes preceded by a ^ character. When the editor encounters such a code, it interprets this code as an instruction to extract information from the data slot of the linked spectral frame, and to substitute the information by the code.

If you edit the table by means of the *Edit* command from the pop-up menu, you will see the actual codes which the meta string consists of.

3.9.3.7 Adding table and modifying table frame

A table can be created by using table frames. By default, tables consist of 2 columns and 2 rows. The default number of columns and rows can be changed.

To add a table...

1   ...click on the icon 📇 in the toolbar.

2   Draw a frame on the drawing area by using the left mouse button. The table consists of two columns and two rows.

To add text to a table...

1   ...right click on the position desired in the table.
2   Select the *Edit* command from the pop-up menu.
3   Now, you are directly in the table cell to enter text. **When editing table cells you can change between the different cells by using the tab key.**

To modify the table frame...

1   ...right click into the table frame.
2   Select the *Properties* command from the pop-up menu.
3   The *Table Properties* dialog opens.
4   Use the different tabs of this dialog to define general settings for the table frame.
5   To confirm the settings click on the *OK* button.

The *Parameters* and *Formats* tabs of the *Table Properties* dialog are described in the following. For details on the *Item* tab refer to chapter 3.9.3.5.
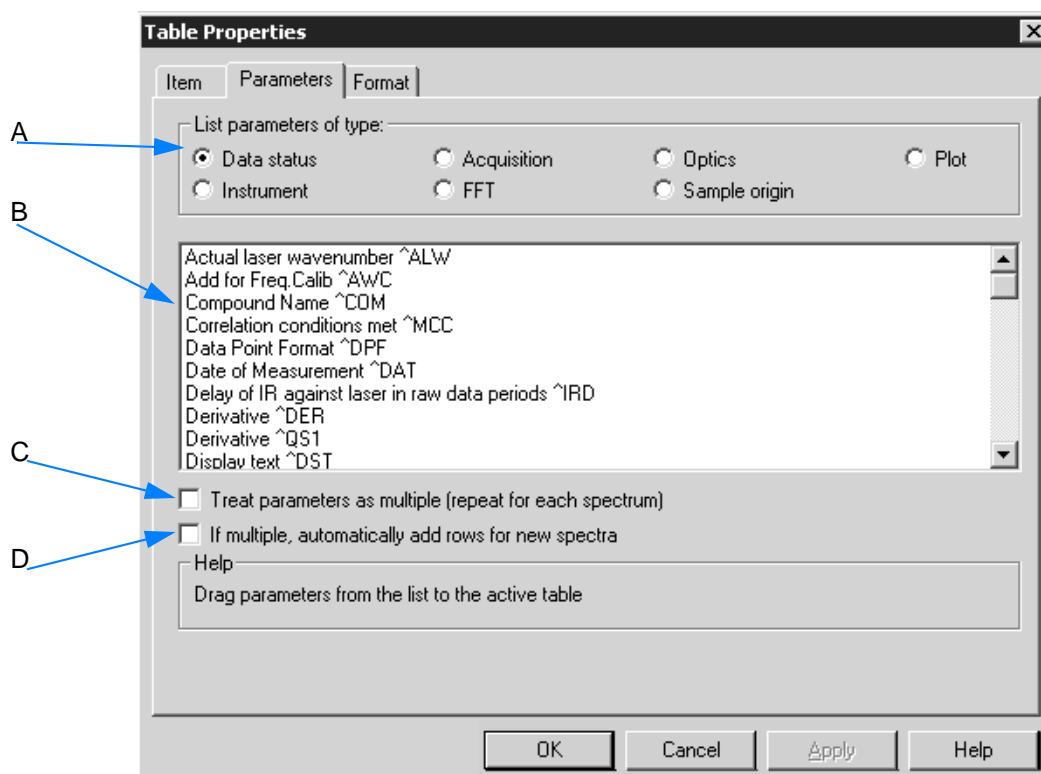
Figure 211: Table Properties - Parameters tab

A Different types of parameters are available. Select one of them.

B The entries of the list box depend on the type of parameter selected (A). To add information to a table, select an item from this drop-down list and drag & drop it to the particular table cell.

The entries in the list box are meta strings, i.e. three-letter codes preceded by a ^ character. When the editor encounters such a code, it interprets this code as an instruction to extract information from the data slot of the linked spectral frame, and to substitute the information by the code.

If you edit the table by means of the *Edit* command from the pop-up menu, you will see the actual codes which the meta string consists of.

C Normally, the information extracted by the editor to expand the meta strings is taken from the corresponding spectral frame in Slot 1. If you activate the *Treat Parameters as Multiple* check box, the parameters will be repeated for each spectrum within a particular frame until the maximum number of rows defined on the *Format* tab has been reached. A separate table cell is available for each spectrum within the table frame.

D The more spectra you add to a frame, the more additional table cells can be created to be able to display the parameters for each spectrum. If you activate the *If Multiple, automatically add rows for new spectra* check box, the number of rows set on the *Format* tab will become meaningless.

Format
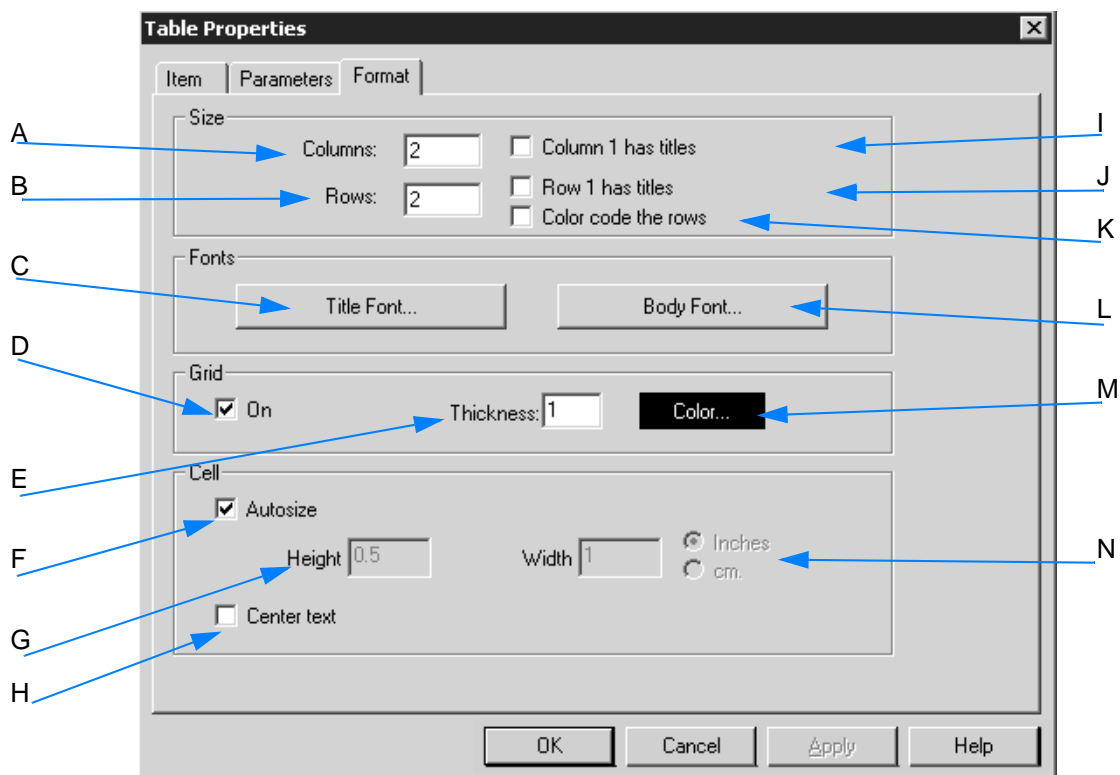
Figure 212: Table Properties - Format tab

A   Define the number of columns included in the table. The default setting is 2 columns.

B   Define the number of rows included in the table. The default setting is 2 rows.

C   Use the button to determine the font for the title. Make sure that you first activate the *Row 1 has titles* check box.

D   If you activate the check box, a grid is displayed around each table cell for better distinction.

E   The value entered into the entry field determines the thickness of the grid in pixels.

F   If you activate the check box, cells will automatically be adjusted to the size of the table frame.

G   If you do not activate the check box, define the height and width of the cells by means of the two entry fields according to the unit specified (M).

H   Activate the check box if you want to center text within the table.

I   If you activate this check box, the text in **column 1** is used as column header, and displayed in the font specified by the *Title Font* button (C).

J   If you activate this check box, the text in **row 1** is used as row header, and displayed in the font specified by the *Title Font* button (C).

K   To better distinguish the rows you can activate the check box. The parameters will then be displayed by the corresponding spectral color.

L   The button allows to specify the body font for the table text. This font applies to all table cells, provided you have not activated the *Column 1 has titles* (I) and *Row 1 has titles* (J) check boxes.

M   The button allows to specify the color of the grid to be displayed. If you click on the button, a color palette opens. Select or define the color desired. The *Color* button will be displayed in this color.

N   Define the unit for the height and width of table cells if you have not activated the *Autosize* (F) check box.

3.9.4   Open Layout

Definition	The *Open Layout* command shows a list of existing templates.
Principle	When using this command for the first time after the OPUS installation you have to navigate to the particular directory. By default, templates are stored in *C:\Program\OPUS* and have the file extension **.PLE*.

3.9.5 Print 🖨/Print Preview

Definition	You can view the result of a printout using the *Print Preview* command. The *Print* command starts printing immediately.

3.9.6 Print Setup

Definition	Use the *Print Setup* command to define the printer and the print parameters, e.g. paper size and print quality. Clicking on the *Properties* button opens a different dialog which can be used to perform further settings depending on the printer configuration.

3.10 Macro

For certain regular procedures you can create a procedure by using the macro wizard. This kind of OPUS macro is a procedure of OPUS commands which are executed all in one.
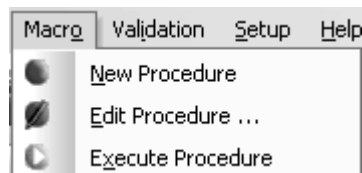
Figure 213: Macro menu

3.10.7 New Procedure ⚫

Definition	The *New Procedure* command allows to create a specific procedure to automate simple sequences of events.
Principle	When creating such a procedure you can either follow the on-screen instructions provided by the macro wizard, or click on single OPUS icons in the OPUS wizard, toolbar or *Macro* menu. to define the procedure manually. **Procedures are stored as Visual Basic Scripts and have the file extension** ***.obs.**

When selecting the *New Procedure* command, a separate view opens.
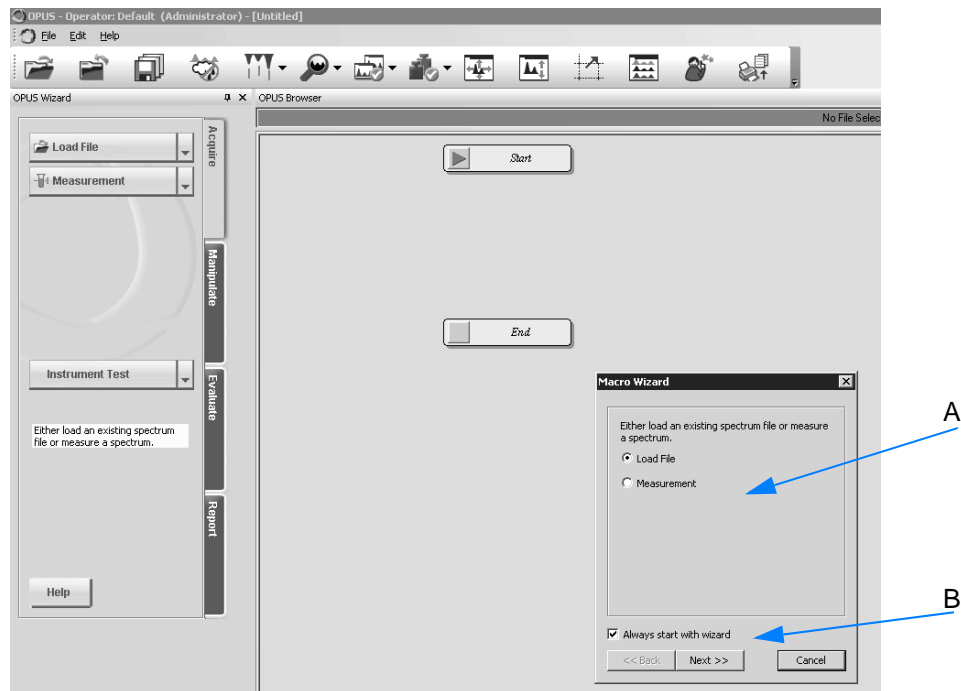
Figure 214: New procedure view

By default, the macro wizard (A in figure 214) is displayed in this view. If you want to change this default setting, deactivate the *Always start with wizard* check box (B). In this case you have to define the procedure manually.

Creating procedure manually

1   Click on the desired OPUS command in the OPUS wizard.

2   The OPUS command is automatically added to the new procedure view in the form of a procedure block.

3   Double clicking on a procedure block opens the corresponding OPUS command dialog. Use this dialog to adjust the parameters for the respective procedure block.

4   To delete a certain procedure block, left click on the block and press the *Del* key on the keyboard.

5   To store a complete procedure created right click into the view and select the *Macro → Save* option from the pop-up menu (see chapter 3.10.7.1).

Working with the macro wizard

The macro wizard facilitates creating procedures. Select the commands used for a particular procedure from the macro wizard.

Step 1:

Define whether you want to load a file or perform a measurement block in case of the first procedure step. If you click on the *Next* button (A in figure 215), the corresponding procedure block is added to the graphical view.
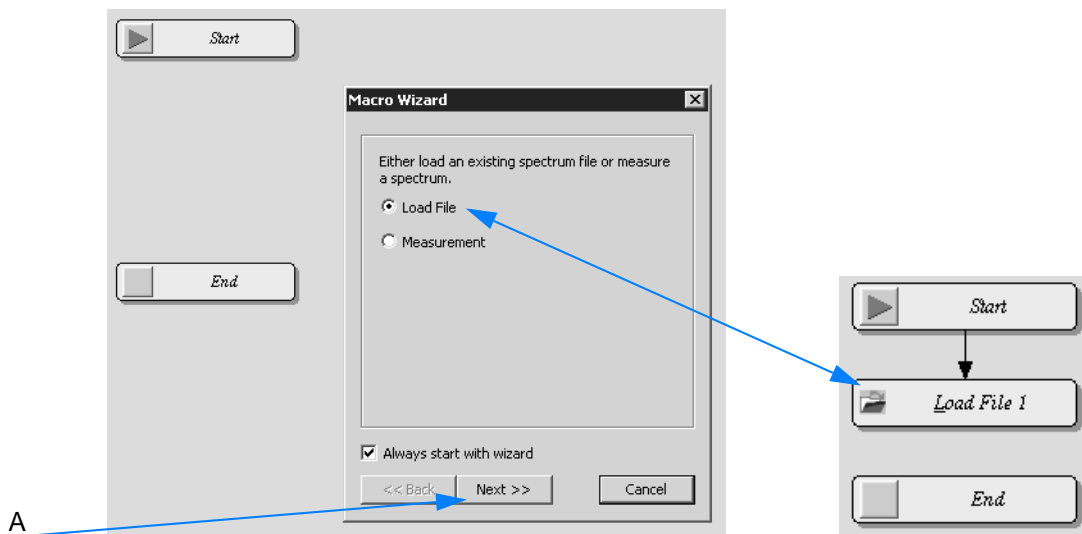
Figure 215: Macro wizard - Load file

Step 2:

Define a manipulation command for the next procedure step. The *Other* drop-down list includes additional manipulation commands. If you click on the *Next* button, the corresponding procedure block is added to the graphical view.
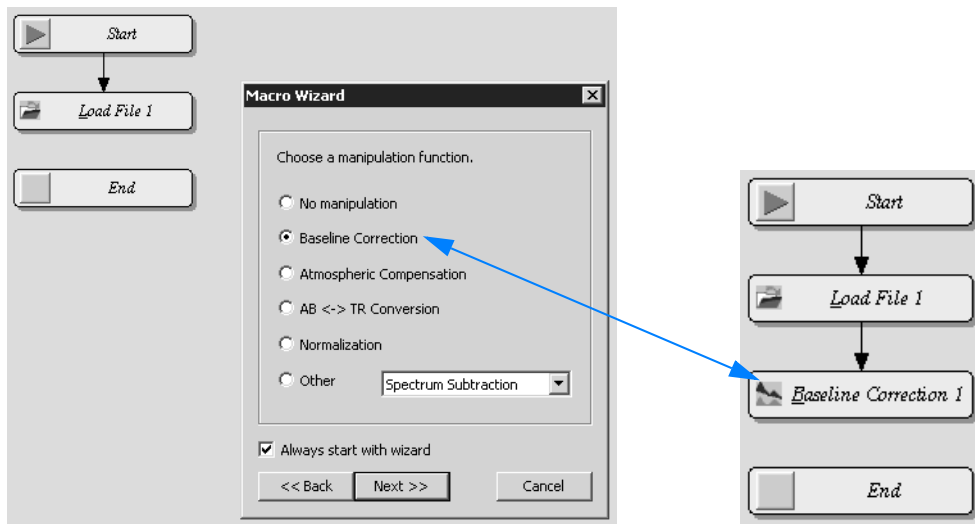
Figure 216: Macro wizard - Manipulation commands

After selecting a manipulation command and clicking on the *Next* button, the *No manipulation* option button is activated by default in the next dialog.
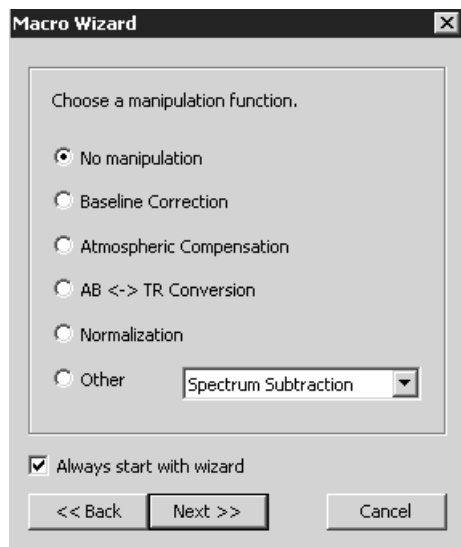
Figure 217: Macro wizard - No manipulation

Note: To add further manipulation commands check the respective option button before clicking on the *Next* button.

Step 3:

Define an evaluation command for the next procedure step. The *Other* drop-down list includes additional evaluation commands. If you click on the *Next* button, the corresponding procedure block is added to the graphical view.
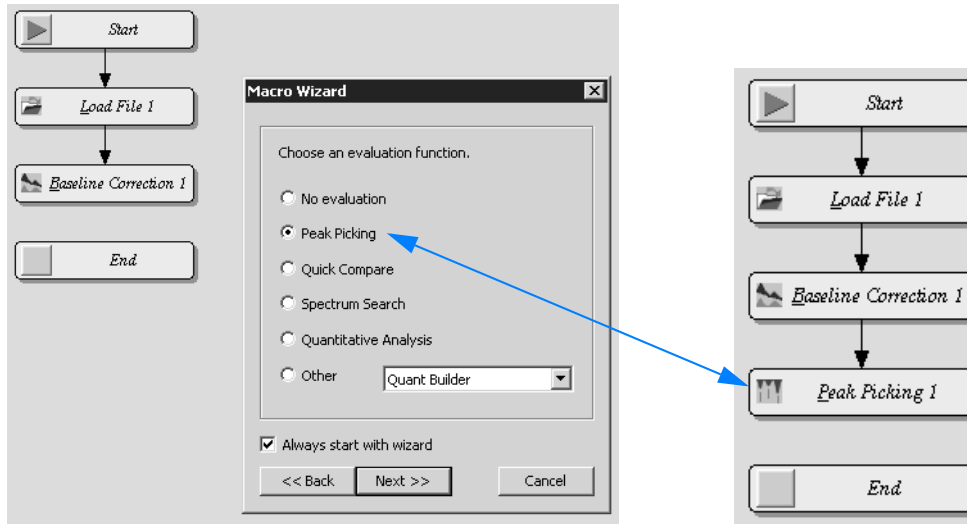
Figure 218: Macro wizard - Evaluation command

After selecting an evaluation command and clicking on the *Next* button, the *No evaluation* option button is activated by default in the next dialog.
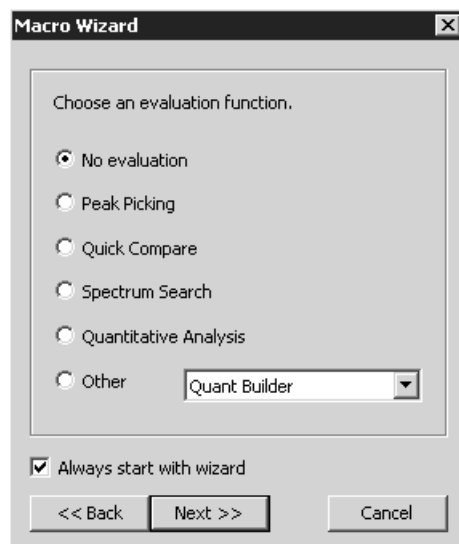
Figure 219: Macro wizard - No evaluation

Note: To add further evaluation commands check the respective option button before clicking on the *Next* button.

Step 4:

For the last procedure step define whether the file is to be saved or printed. If you activate the *Loop* check box the procedure previously defined will be repeated *n* times.

If all settings are made, click on the *Finish* button. The complete macro procedure created is displayed.
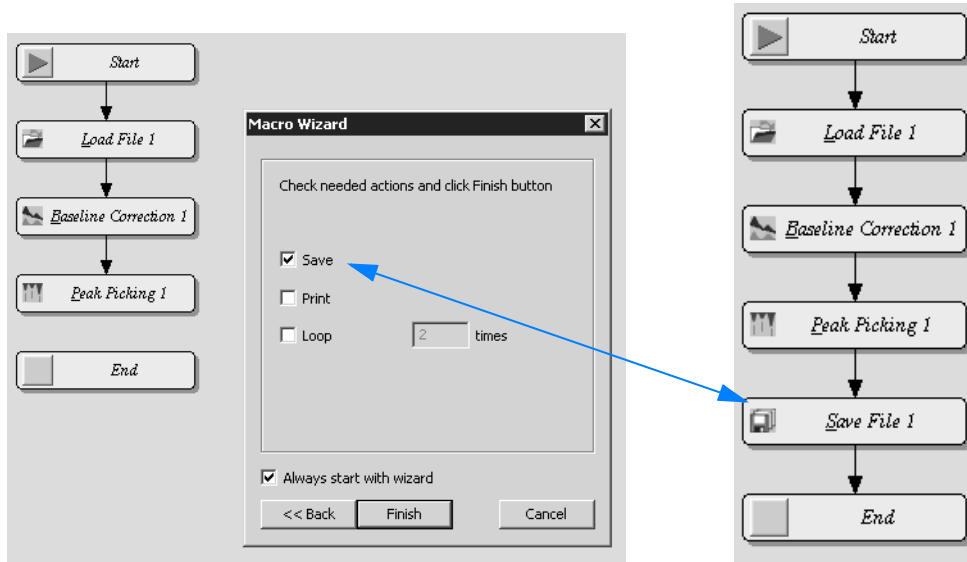
Figure 220: Macro wizard - Save, print; complete procedure

Double click on the procedure block **to define the parameters** for the respective block. The OPUS command dialog opens which allows to set the parameters for the block selected.

Left click on the block and press the *Del* key on the keyboard **to delete a procedure block**.

To store the complete procedure right click onto the procedure view. Select the *Macro → Save* command from the pop-up menu (see chapter 3.10.7.1).

3.10.7.1 Pop-up menu

Right clicking somewhere on the procedure view opens a pop-up menu which consists of the following commands:

Figure 221: Pop-up menu

The pop-up menu commands can be used to edit, check or save the procedure created. In the following each of the commands will be described in more detail.

Macro
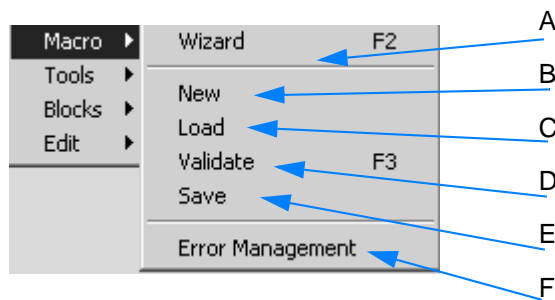
Figure 222: Pop-up menu - Macro

A Starts the macro wizard.

B Opens a new procedure workspace.

C Loads existing procedure.

D Allows to check the procedure created, i.e. it will be checked whether the course of actions within the procedure is valid. If not, a message box pops up indicating how the existing procedure has to be modified, as the following example shows:
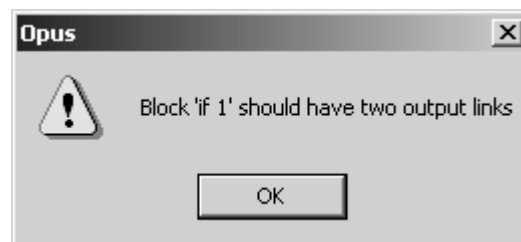
E Saves the procedure. Define the file name and directory path in the dialog displayed. **The macro procedure is stored as OPUS basic script and has the file extension *.obs.**

F This is a global setting which specifies how the script should react in case of an error. If you click on *Error Management*, the following dialog opens:
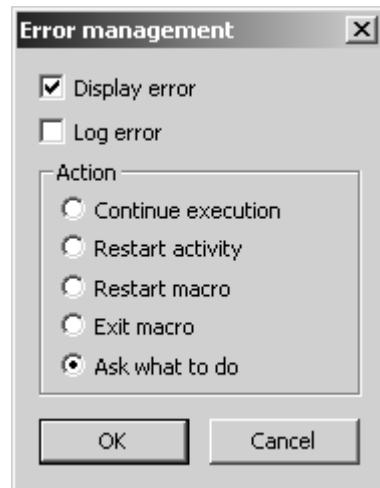
Activate the appropriate check box or option button to further define the error management.

Tools
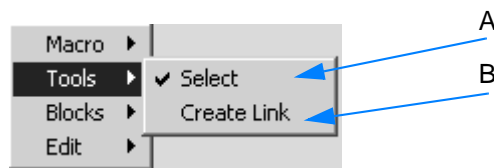
Figure 223: Pop-up menu - Tools

A Allows to select a certain procedure block. This option is checked by default. To select a procedure block, left click on it, and it will be marked by a broken line:
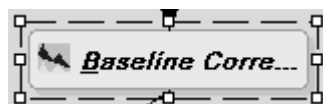
Now, you can move any procedure block to a different place if you press and hold down the left mouse button. When positioning a procedure block on a black connecting arrow between two different procedure blocks, this arrow becomes red, visualizing that you are now changing the original procedure structure. As soon as you release the mouse button the procedure block moved will exactly be positioned between these two different procedure blocks.

B Explicitly creates an arrow link, e.g. in case of *IF* procedure blocks. To delete a link, click on the arrow which turns red and press the *Del* key on the keyboard.

Blocks
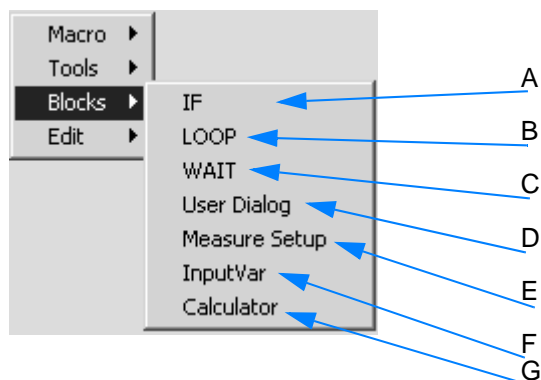
Figure 224: Pop-up menu - Blocks

A Creates an *IF* procedure block which always requires two output
   links. If you integrate the *IF* block into an existing procedure, the
   following dialog opens:
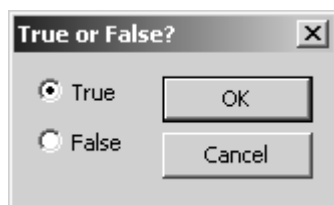
Specify which condition, i.e. *True* or *False* has to be used to con-
tinue. Double clicking on an *IF* procedure block displays the follow-
ing dialog:
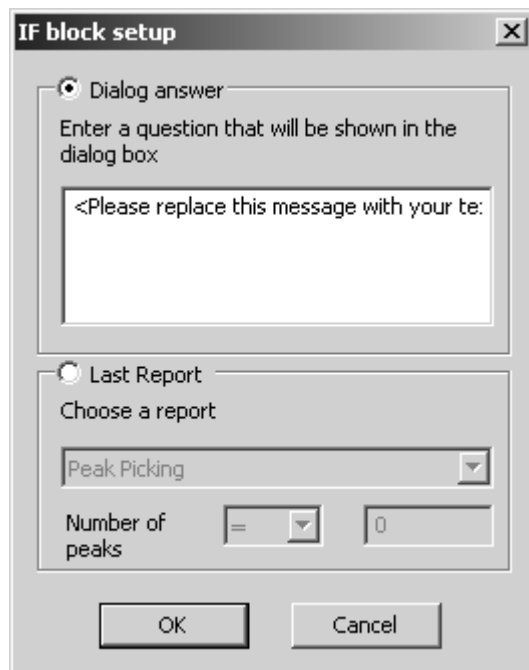
If you activate the *Dialog answer* option button, you have to enter
an appropriate question into the entry field. You can also define
whether the *IF* block shall be based on a previous evaluation
report.

Depending on the report selected from the drop-down list further details can be defined with regard to the condition. If you have, e.g., selected *Peak Picking*, you can further determine whether the number of peaks should be [ ] than the number specified in the entry field. In case of a *Search* report the value to compare with will be the hit quality.

B Creates a *LOOP* procedure block. This kind of procedure block is used to repeat certain commands. Define the loop count in the dialog that pops up when double clicking on the *LOOP* procedure block.
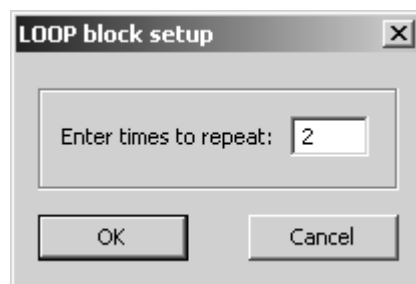
C Creates a *WAIT* procedure block. This kind of procedure block is used to interrupt the current course of action. The period of time can be exactly defined in the dialog that pops up when double clicking on the *WAIT* procedure block.

D Creates a *Message Box* procedure block. To manually enter the text double click on the *Message Box* procedure block.
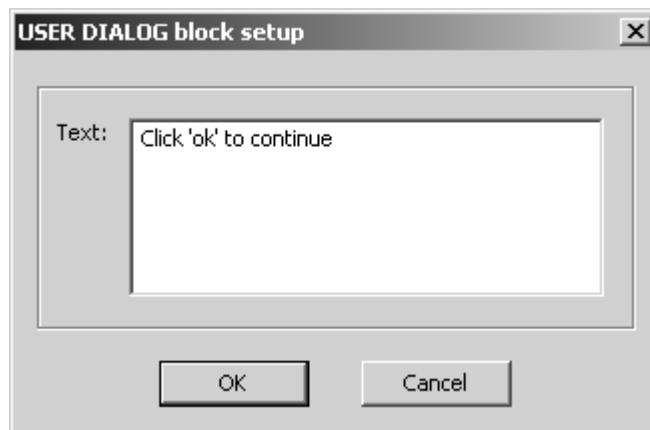
E Creates a *QUICK MEASURE* procedure block. If you integrate such a block into the procedure, specific parameters will be prompted when running the macro. To explicitly define these parameters double click on the *QUICK MEASURE* procedure block.
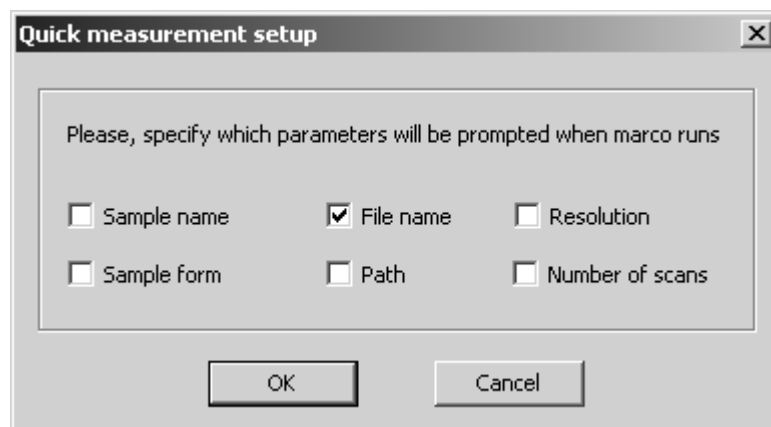
F Creates the *Input Variable* procedure block. Enter the name and the default value of the variable by double clicking on the *Input Variable* procedure block.
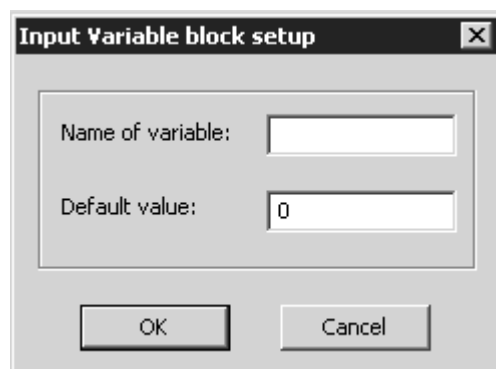
G Creates the *Calculate* procedure block. This block can be used to perform calculations on the basis of evaluation results. OPUS provides pre-defined variables. Double click on the *Calculate* procedure block.
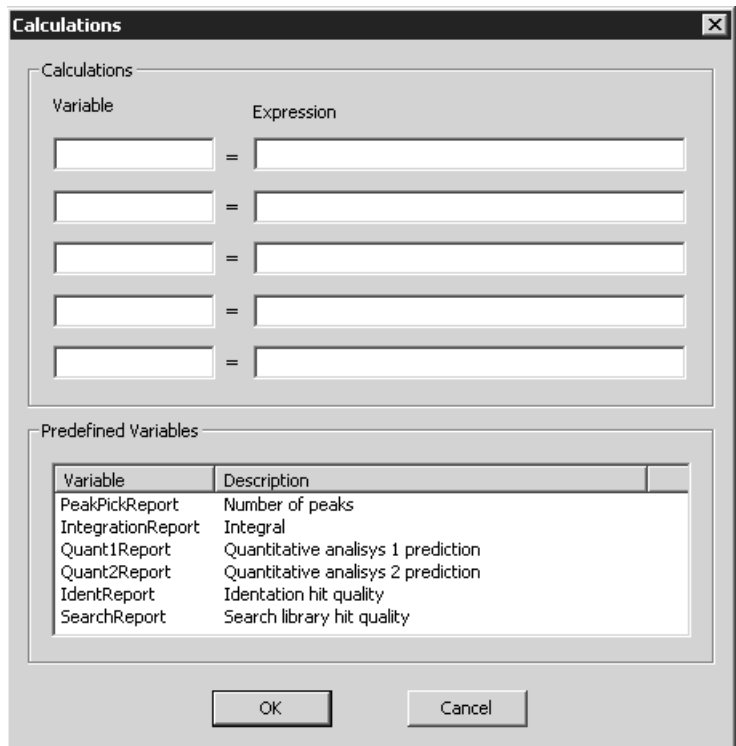
Enter the name of the variable into the *Variable* entry field. The predefined names of each variable as well as the description of the corresponding variable value are included in the list below. Enter the mathematical term for the variable defined into the *Expression* entry field. **Example:**
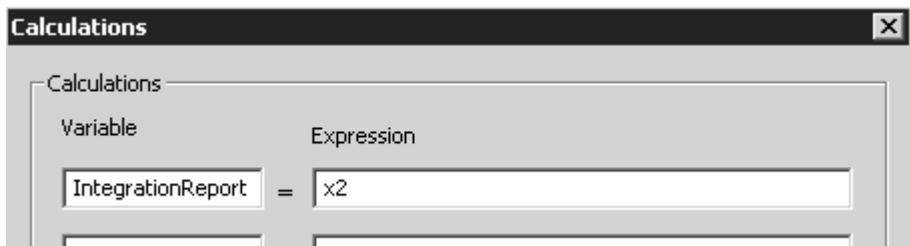
Edit
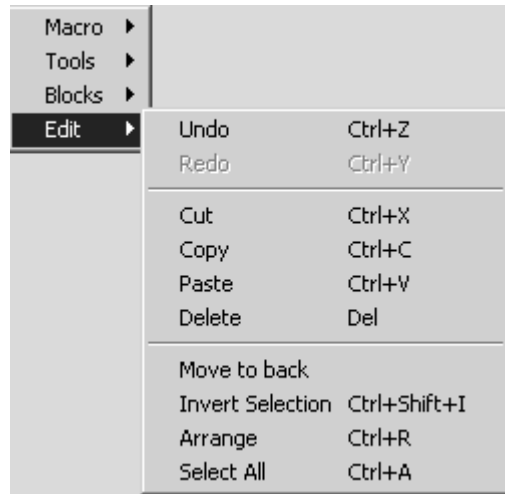
Figure 225: Pop-up menu - Edit

- **Move to back:** in case of two procedure blocks on the same position moves the one selected behind the other
- **Invert selection:** inverts the procedure selected
- **Arrange:** arranges the procedure
- **Select All:** selects all procedure blocks

3.10.8 Edit Procedure

Definition	The *Edit Procedure* command allows to edit a procedure created.
Principle	Select the command. A dialog opens which you select the respective procedure from. **Procedure files have the extension *.obs.**

3.10.9 Run Procedure

Definition	The *Run Procedure* command allows to start a procedure created.
Principle	Select the command. A dialog opens which you select the respective procedure from. **Procedure files have the extension *.obs.**

3.11   Validation

The *Validation* menu allows to retrieve the parameter settings of the instrument test. Measurement and test parameters are stored in a set of databases which have been installed when installing OPUS.

> **Note: If you have received a separate database CD, you also have to install this CD.**

Furthermore, the *Validation* menu allows to start the instrument test and define the optic parameters.

Figure 226: Validation Menu

3.11.1 Setup Instrument Test[1]

Definition	Use the *Setup Instrument Test* command to retrieve the standard instrument test settings, and measure the laser wavenumber.
Principle	An instrument test consists of several single tests and qualifies spectrometer performance in daily routine work. The active test channel (sample compartment or ATR) is automatically defined and assigned to the instrument test. A measuring configuration with individual parameter settings are specified for each channel.

If you select the *Setup Instrument Test* command, the automatically pre-defined measuring configuration for the active test channel is shown.

> **Note: The pre-defined settings for the test channel and instrument configuration as well as the accessory must not be changed!**

Figure 227 exemplifies the *Sample Compartment* test channel for ALPHA-T (transmission unit).

---

1. In some cases OPUS also uses OVP (OPUS Validation Program) as reference with regard to the command used to set and perform the instrument test. The instrument test itself is sometimes called PQ test (Performance Qualification).
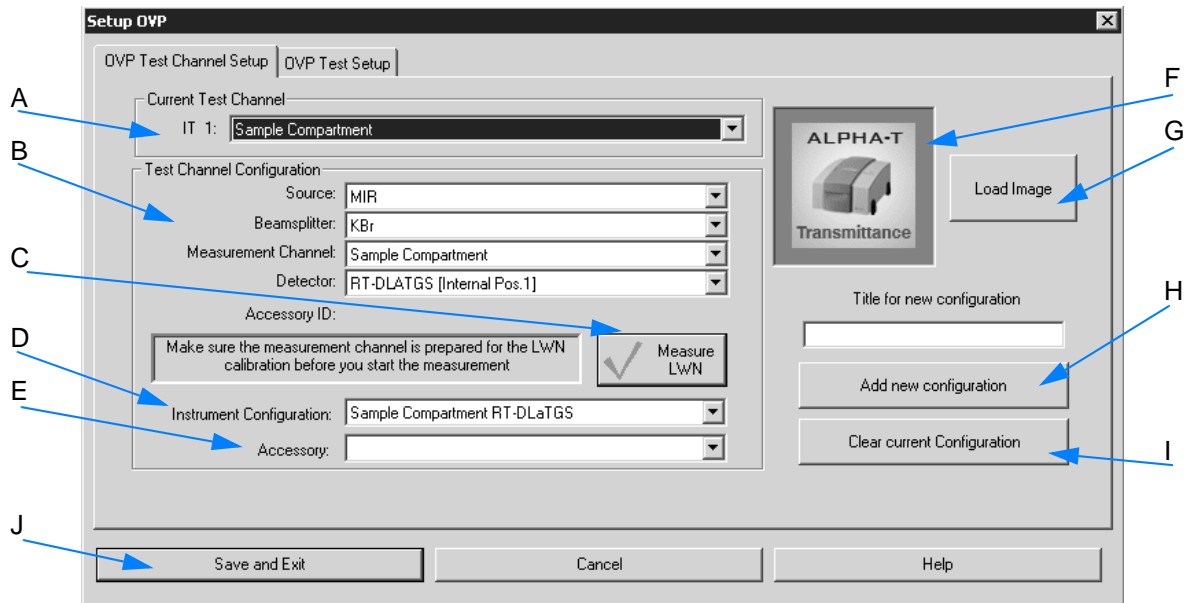
Figure 227: Test channel setup

A   The drop-down list shows the test channel used.

B   For each spectrometer test channel a measuring configuration is pre-defined. This configuration is used during actual validation measurement and is a valid combination of source, beam splitter, measurement channel and detector.

The settings are made by default for each drop-down list. According to these settings the appropriate instrument configuration (D) and the bitmap (F) specified for the measurement channel will automatically be displayed.

C   Click on this button to set up the laser wavenumber. See also chapter 3.11.1.2.

D   The instrument configuration is automatically displayed according to (B).

E   Depending on the test channel (A) specified, the drop-down list contains appropriate accessories. The following example shows a list of ATR accessories:
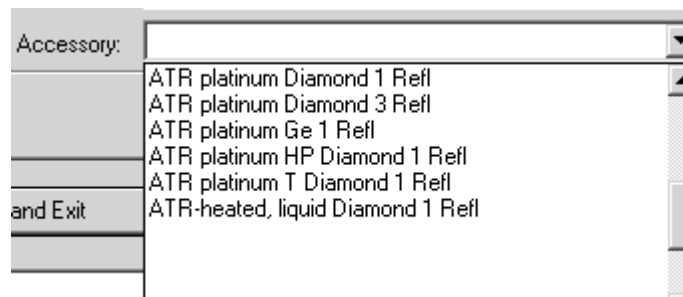
Figure 228: List of ATR accessories

In case of ALPHA-T the *Accessory* selection field is empty.

F Depending on the measurement channel or accessory selected a configuration-specific bitmap is displayed.

G Use the *Load Image* button to load further instrument images available in OPUS (see chapter 3.11.1.1). The bitmaps are stored in the *OPUS\VALIDATION\Bitmaps* directory. **Note: Select the *Thumbnail* option from the pop-up menu by clicking on the** **button to be able to see at once which bitmap belongs to which file name.**
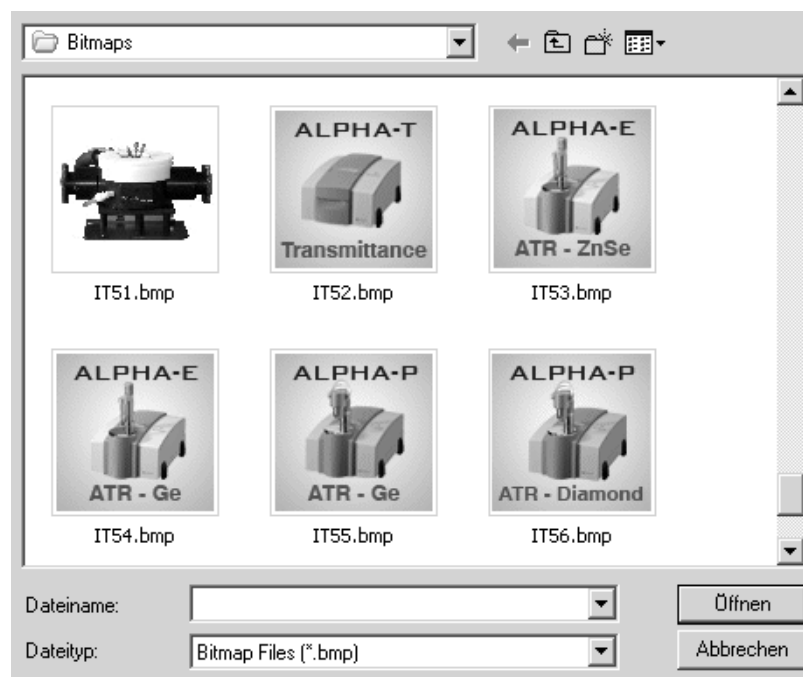
Figure 229: Instrument Bitmaps

You can also make your own photo with a size of 90 x 90 and store it into the bitmap directory using the *ITnn.* file name (*nn* is a consecutive number).

H This button is only provided for instruments which do not support the automatic test channel setup. **As ALPHA supports the automatic test channel configuration you must not use this button to add a new test channel configuration!**

I This button is only provided for instruments which do not support the automatic test channel setup. **As ALPHA supports the automatic test channel configuration you must not use this button to delete the current test channel configuration!**

J To save the configuration click on the *Save and Exit* button.

3.11.1.1 Instrument test bitmaps

The following bitmaps are used for the different instrument configurations:

	IT52.bmp: ALPHA-T (Transmission)
	IT53.bmp: ALPHA-E, ATR-ZnSe (Zinc selenide crystal)
	IT54.bmp: ALPHA-E, ATR-Ge (Germanium crystal)
	IT55.bmp: ALPHA-P, ATR-Ge (Germanium crystal)
	IT56.bmp: ALPHA-P, ATR-Diamond (Diamond crystal)
	IT56.bmp: ALPHA-R, DRIFT (Diffuse reflection)

3.11.1.2 Measure laser wavenumber

Before starting the instrument test for the current configuration you may first have to calibrate the laser wavenumber (LWN).

Measuring and assigning the laser wavenumber for the current test channel ensures the wavenumber accuracy of spectral data.

> **Note: When starting OPUS for the first time the calibration is automatically performed. Otherwise, you will be prompted to perform a laser wavenumber calibration within regular time intervals (see also chapter 10.3).**

When is a laser wavenumber calibration required?

1   At the initial instrument operation. In this case the laser wavenumber calibration runs automatically.

2   If OPUS prompts you to perform a laser wavenumber calibration.
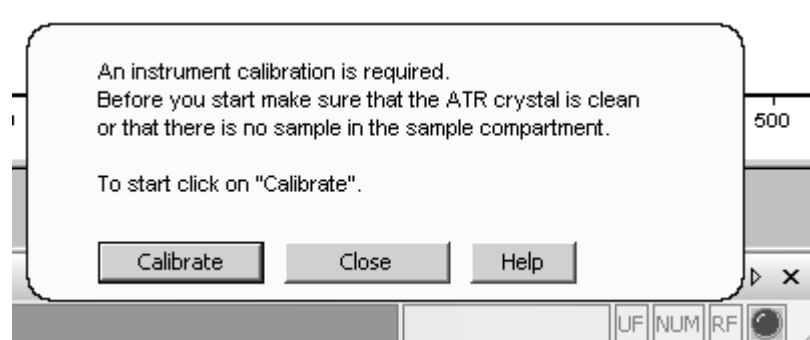
Figure 230: Request to calibrate laser wavenumber

To calibrate the laser wavenumber...

...click on the [Measure LWN] button. A laser wavenumber calibration is only valid for the accessory currently connected. Therefore, first select the appropriate test channel from the *Current Test Channel* drop-down list (A in figure 227). If the test channel selected is not suited for the accessory, the following error message pops up:

Figure 231: Error message in case of wrong test channel

When calibrating...

... a spectrum of water vapor is measured. A specific water band is used to determine the optimum laser wavenumber.

To verify the validity of the water band adjacent water bands are checked as well. In a second step the appropriate wavenumber is verified against the bands of the polystyrene filter on the internal validation unit.

After calibration...

...a result dialog pops up.
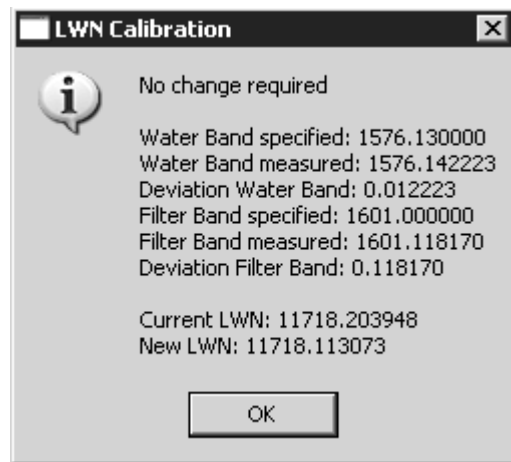
Figure 232: LWN calibration result

The LWN test result shows the water bands specified and measured. You can also see the water band deviation as well as the laser wavenumber, i.e. both the specified and newly calculated one.

If the current LWN for a particular channel is within a certain tolerance, the test has passed and no further changes are required.

If the deviation is beyond a certain tolerance, the LWN value for the current measurement channel is set to the currently computed optimal value when clicking on the *OK* button. Now, a green check mark is added to the [Measure LWN] button.

If the laser wavenumber calibration has not passed...

...the water vapor concentration of your instrument may be too low or too high, and a warning pops up.

In this case check the *LWN_Water.x* water vapor spectrum (with *x* being any number) which is located in the *OPUS\VALIDATION\DATA\LWNCalibration\<Date>\<Time>*[1] directory.

---

1. Date: YYYYMMDD (year/month/date); Time: HHMMSS (hour/minute/second)

Water vapor concentration	What is to be done?
Too low	Remove the desiccant cartridge for a short period of time to allow the water vapor concentration in the instrument to increase. See chapter 9.2
Too high	Replace the desiccant cartridge, see chapter 9.2.

In both cases repeat the measurement until the result is *OK* (also see chapter 3.11.1.4).

3.11.1.3 OVP test setup

The instrument test parameters are displayed on the *OVP Test Setup* tab.
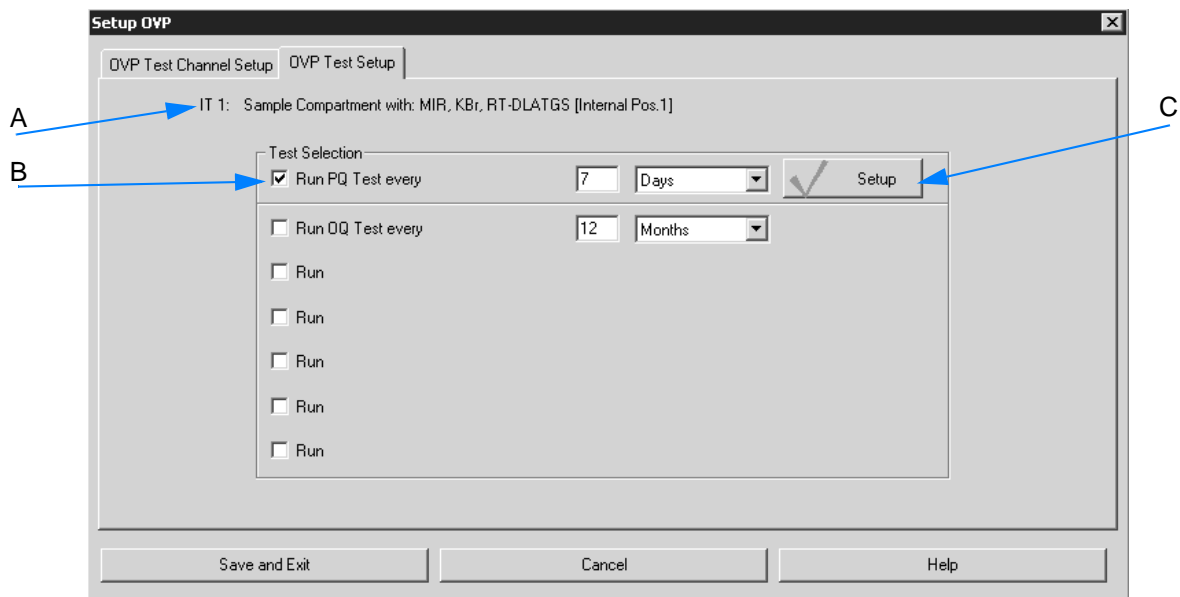
Figure 233: Instrument test parameters

A Test channel currently selected is displayed.

B The check box is activated by default. It is recommended to repeat the instrument test within a certain time interval. The time interval for the instrument test is set to 7 days by default.

To specify a different interval type the interval period into the entry field and select the units from the drop-down list. Available units are hours, days, or months.

C Clicking on this button opens another dialog. This dialog shows the different tests which belong to the instrument test.
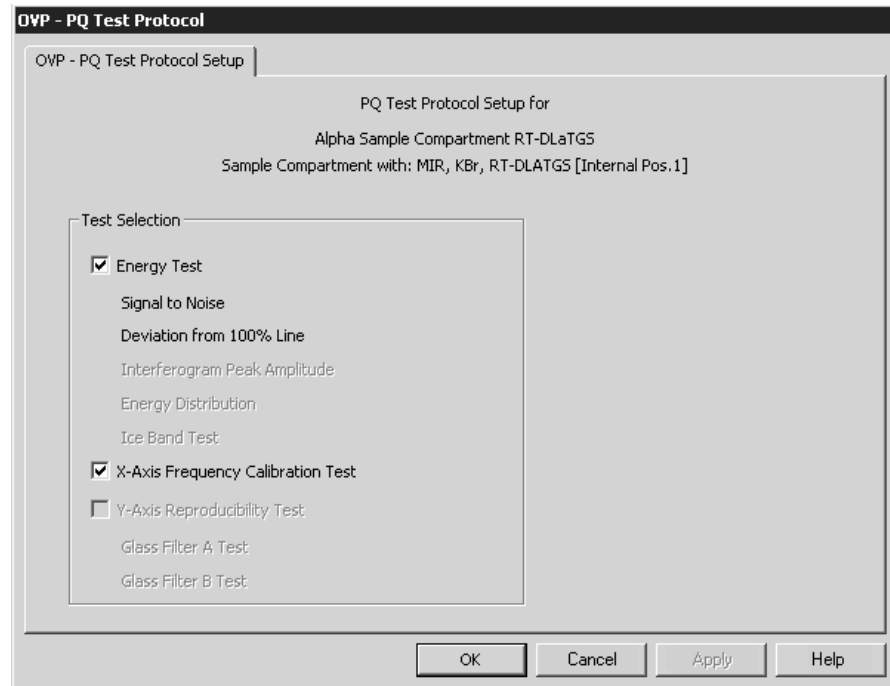
Figure 234: Single tests

All tests available are checked by default. In exceptional cases (not recommended) you can deactivate certain tests by removing the check mark.

3.11.1.4 Single-test description

The instrument test consists of different single tests which are set by default. These tests are described in the following.

Energy Test	Signal-to-Noise	Verifies that the signal-to-noise ratio is better than a specified limit.
	Deviation from 100% Line	Verifies that the 100% line does not shift on long term.
X-Axis Frequency Calibration Test		Verifies that the frequency calibration of the instrument is correct.

Signal to Noise (S/N) Ratio

The signal-to-noise ratio test determines the sensitivity of the spectrometer by calculating the average signal-to-noise ratio of ten 100% spectra.

The S/N ratio is determined by collecting and analyzing a 100% spectrum. A 100% spectrum is the ratio of two successively acquired single-channel spectra with no sample in the sample compartment. The ratio of these two single-channel spectra is used to generate a transmission spectrum.

The S/N ratio is calculated by the OPUS *Signal-to-Noise Ratio* command in the *Evaluate* menu, using peak-to-peak by means of the quadratic parabola fit option. In order to get a reliable result 10 spectra are measured (reference and sample).

The S/N ratio is calculated separately for each of the spectra. For the test the mean value of all 10 results is used.

Figure 235 shows a peak-to-peak noise of 0.1%, referring to 100% transmittance in MIR region. To calculate the S/N ratio the reciprocal value is multiplied by 100 (1 / 0.1 * 100).
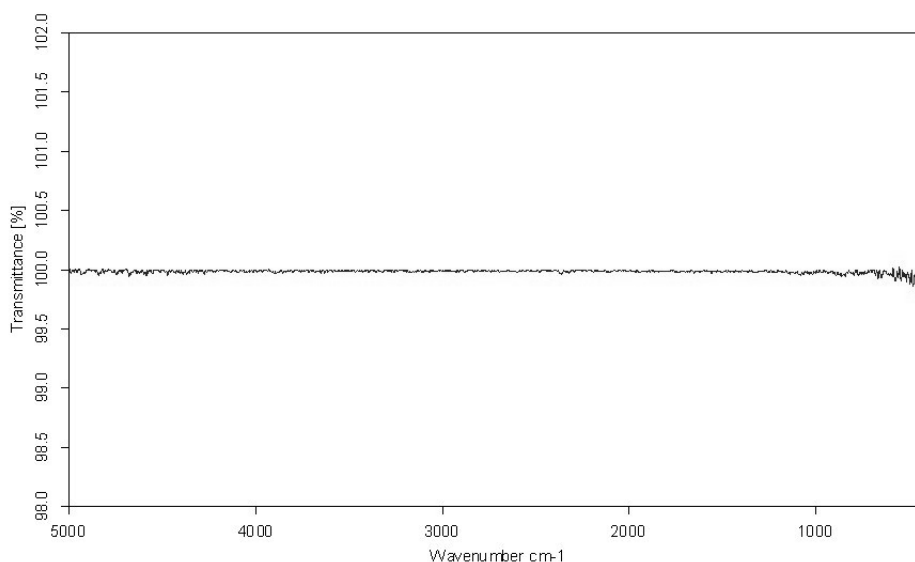
Figure 235: MIR 100% line

Deviation from 100% Line

This test measures the maximum deviation of a 100% line within a larger frequency range.

The average determined by 10 measurements must not exceed the predefined limit.

X-Axis Frequency Calibration Test (Wavenumber accuracy)

The x-axis frequency calibration test ensures that the frequency calibration of the instrument is within the specified limits. To determine the wavenumber accuracy a polystyrene standard sample is measured. The standard is on the internal validation unit. Thus, no further actions are required for this test.

3.11.2 Run the Instrument Test

Definition	This command allows to start the instrument test.
Principle	The instrument test consists of a test protocol which includes the tests performed. If the test has completed, a pass/fail interface is shown with the option to view or print the detailed report.
	If the test has passed, the OPUS status light will be green. The operator can continue using the spectrometer as the instrument has been properly tested.
	Note: Test spectra and reports are stored in the OPUS standard directory *C:\Program\OPUS\VALIDATION\Data* and *\Reports*.

How to start the instrument test?[1]

1　Select the *Run Instrument Test* command.
2　If the validity period of the test has expired, the *Run PQ-test* check box is activated by default.
3　Define whether a report has to be printed or shown automatically.
4　Click on the *Run Tests* command.

The dialog of this command is described in the following.

---

1. The instrument can also be started by means of the *Instrument Status* dialog or the OPUS wizard. See description in this chapter.
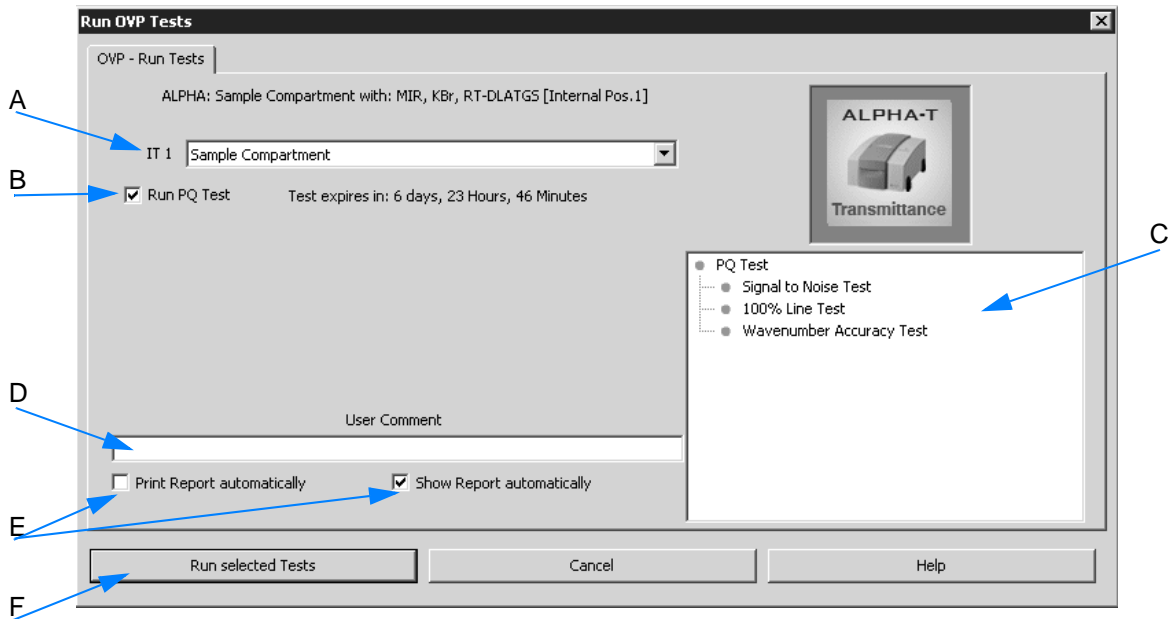
Figure 236: Run instrument test

A The *IT n* drop-down list allows to select the correct test channel required for the accessory currently used.

B Shows the instrument test status. Tests which have expired or which have not yet been performed are automatically activated for measurement. Tests which have not yet expired are not activated, and their remaining time is indicated as a reminder.

If a test has not expired, but the interval has only e.g. 2 hours left you can activate the check box for that test and run the test earlier.

Note: If the instrument test has expired and you do not perform this test, you are not allowed to use this channel in routine environment.

C You can see which test(s) will be performed by the browser-like display next to the bitmap. This kind of display is only available if the check box (B) has been activated before.

D All measurement results are stored in a report (PDF file) and in the *UserData* database. To append a comment to the current test protocol entry write a comment into the *User Comment* entry field.

E To print or have the test report displayed activate the respective check box. See also chapter 3.11.2.2

F Click on the *Run selected Tests* button to start the instrument test.

Start the instrument test by means of the Instrument Status dialog

The *Instrument Status* dialog can be opened by clicking on the status light [image] in the bottom right corner of the OPUS interface. The status light indicates both the hardware status as well as the current test status of the active test channel. The test status is displayed in different colors and can be as follows:

- **Green:** all tests have passed and have not been expired
- **Yellow:** at least one of the tests has expired or has not yet been performed
- **Red:** the last test has failed

Click on the status light to open the *Instrument Status* dialog.
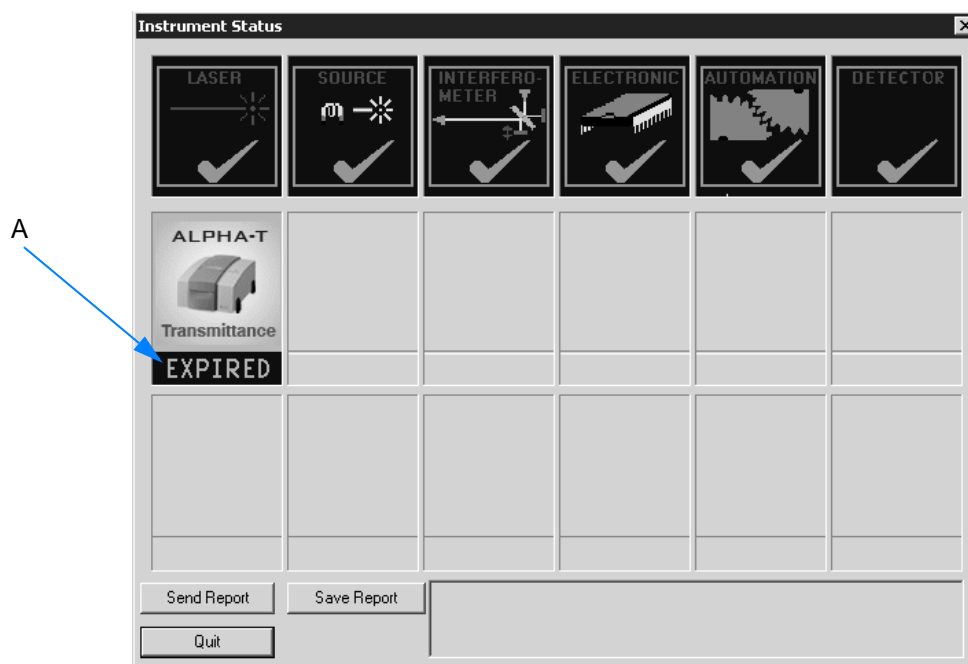
Figure 237: Instrument Status

The test status (A in figure 237) can be indicated as follows:

- **PASSED** (green): test successfully performed and still valid
- **FAILED** (red): test failed
- **EXPIRED** (light-blue): test expired or has not yet been performed

Clicking on the test channel opens the following dialog:
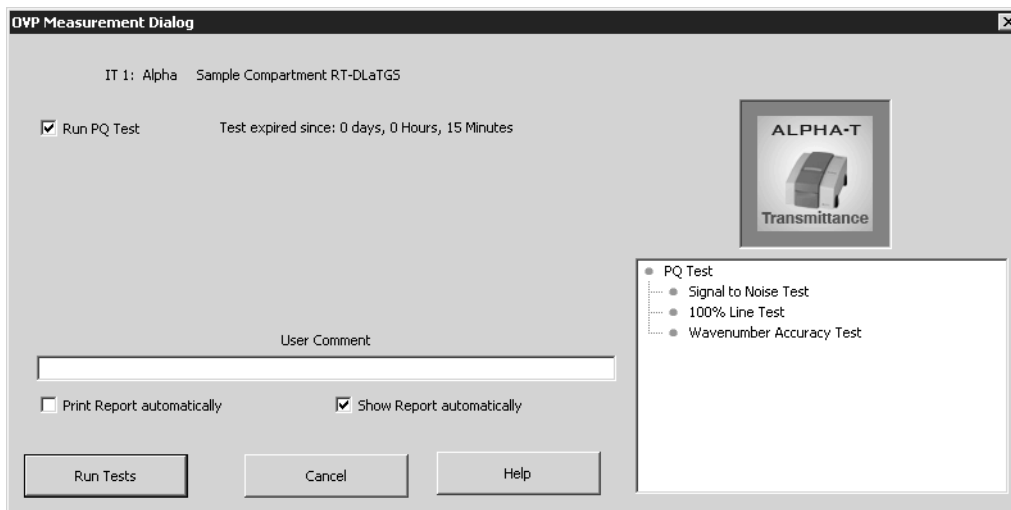
Figure 238: Start instrument test

The *Run PQ Test* check box is automatically activated if a test has expired or failed.

To start the instrument test click on the *Run Tests* button. The dialog closes and the test will run. The status bar indicates different test steps as the following example shows.
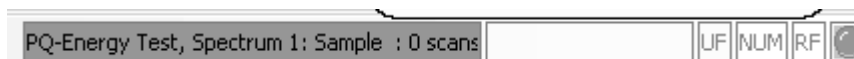
Figure 239: Status bar indicating test is running

If the test has been finished, click on the status light [icon] again at the lower right corner of the spectrum window. The test status has to be *PASSED* now.

Figure 240: Instrument test passed

Start instrument test by means of the OPUS wizard

Click on the *Instrument Test* button in the OPUS wizard. The instrument test starts and runs automatically.
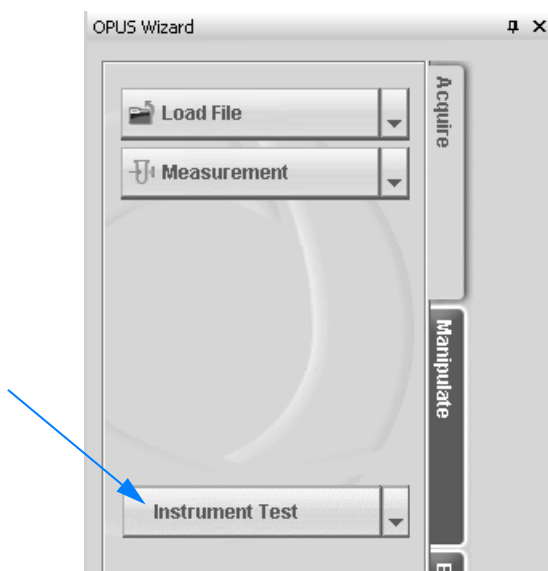
Figure 241: Instrument test in the OPUS wizard

3.11.2.1 Test spectra

The spectra produced when running the tests are stored in a directory structure which will be automatically generated. In the *\Validation\Data* directory a sub-directory is created for the current date, supporting the following format: *YYYYMMDD*[1] (e.g. 20060212). A further sub-directory for the time is created in the directory for the current date, supporting the following format: *HHMMSS*[2] (e.g. 113423).

The spectrum file name always starts with *PQ* and a test name (e.g. *PQ_ALPHA_Sample_Compartment_RTDLaTGSEnergy1.0*). The date and time is also used for the report name to allow a clear correlation between spectra and reports. The spectra contain the test result together with other important data in the ⊞INFO data block.

3.11.2.2 Printing reports

The results of test measurements are stored in a report (PDF format). The test report contains a summarized test result page with all the test spectra and measuring parameters displayed.

---

1. Y: year, M: month, D: day
2. H: hour, M: minute, S: second

Reports are stored in the separate *\VALIDATION\REPORTS* directory and can automatically be printed.

> **Note: To have the report displayed and printed you require the Adobe Acrobat Reader which is available on the OPUS installation CD.**

Figure 242: Test protocol of the instrument test

3.11.2.3 Running instrument test in unattended mode

The internal validation unit (IVU) which is integrated into the spectrometer allows to run, with very few exceptions, the instrument test without any user interaction required.

The *Open Planner* command from the *Setup* menu allows to automatically run the instrument test. For detailed information on the *Open Planner* command refer to chapter 3.12.2.

If the instrument test is to be repeated within a certain time interval, you can define the instrument test as recurring item by using the *Open Planner* command.

To start the unattended mode...

1   ...select the *Open Planner* command from the *Setup* menu.

2   Right click on the respective day and select the *New Appointment* command from the pop-up menu. The following dialog is displayed:

Figure 243: Define instrument test appointment

3   Select the command line required for the accessory connected, e.g. *Run OVP PQ-Test 1: Sample Channel*.

4   Click on the *Recurrence* button. Another dialog opens.

5   Activate the *Weekly* option button as recurrence pattern.

Figure 244: Define recurrence

> 6 Define the start time of the test, either manually or by means of the arrow keys.
>
> 7 Activate the *No end date* option button as range of recurrence.
>
> 8 Confirm your settings by clicking on the *OK* button.

3.11.3 Optic Setup and Service

Definition	The *Optic Setup and Service* command allows to configure the optics and retrieve diagnostic results and statistics of specific spectrometer data.
Principle	Each tab of this command contains different optics features. Define these features and save them.

3.11.3.1 Optical Bench
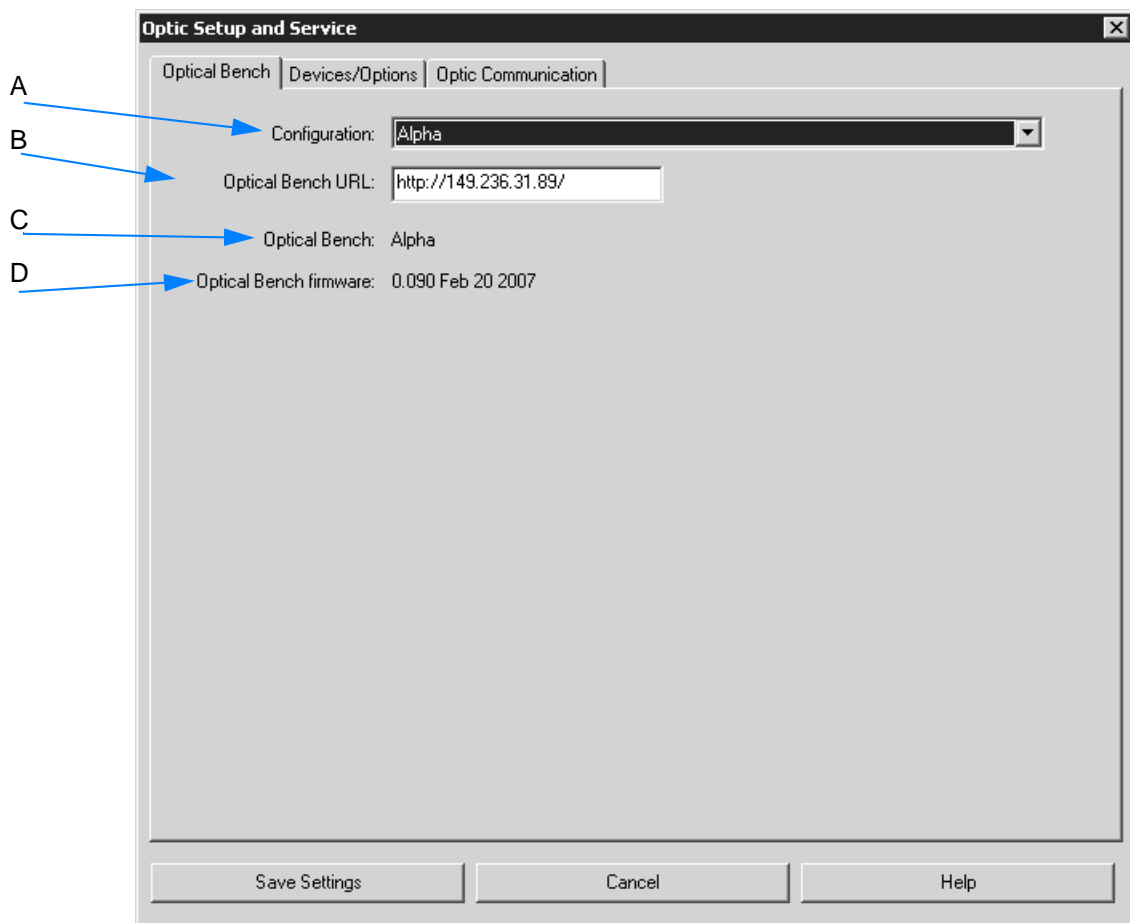
Figure 245: Optic Setup and Service - Optical Bench

A   The drop-down list contains the name of the spectrometer con-
    nected.

B   The URL (Uniform Resource Locator) of the spectrometer con-
    nected is displayed. This URL can be used to access the instru-
    ment   diagnostic   pages   via   an   internet   browser   (see
    chapter 10.3.2).

C   The name of the optical bench (spectrometer) is displayed.

D   The name of the firmware is displayed.

3.11.3.2 Devices/Options

The *Devices/Options* tab allows to configure the spectrometer
components available. All components available for ALPHA are checked
by default.

> **Note: Configuring spectrometer components requires Administra-
> tion user rights in OPUS.**
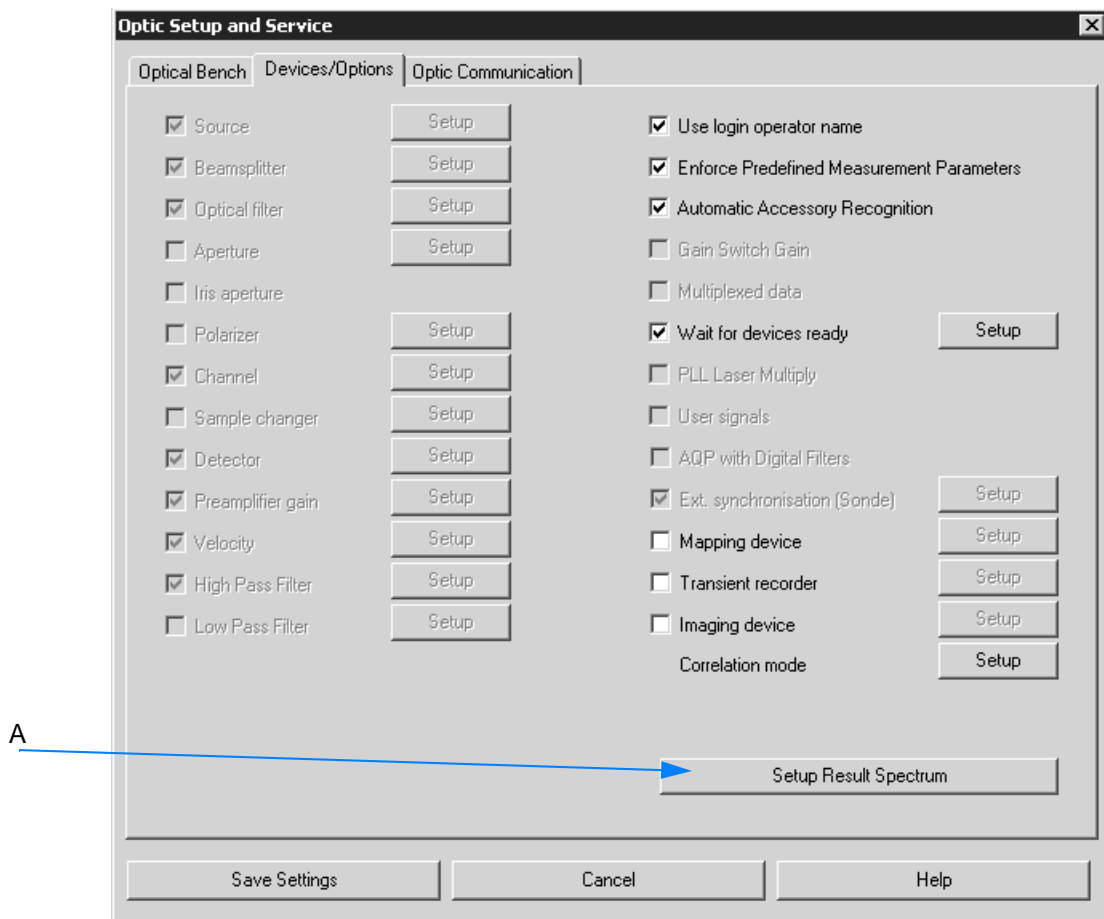
Figure 246: Optic Setup and Service - Devices/Options

To configure the result spectrum...

...click on the *Setup Result Spectrum* button (A in figure 246). As the direct result of a data acquisition is always an interferogram this interferogram can be transformed into spectra of various types, e.g. absorbance, transmittance or reflectance spectra.

A specific result spectrum type is only available in OPUS if the respective result type check box is activated in the following list.
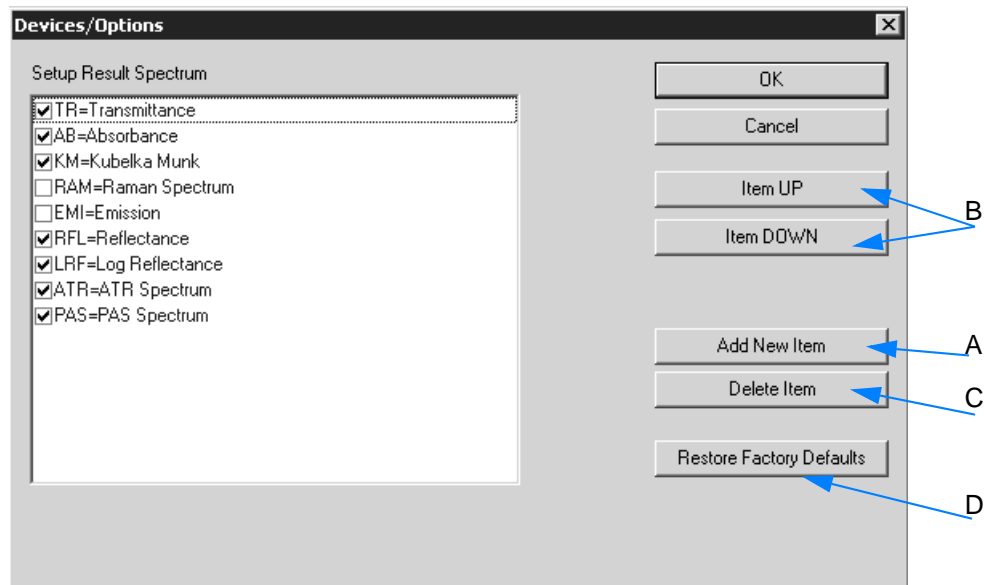
Figure 247: Configuration options of result spectrum

A To add new configuration items click on the *Add New Item* button. A new entry line is displayed.
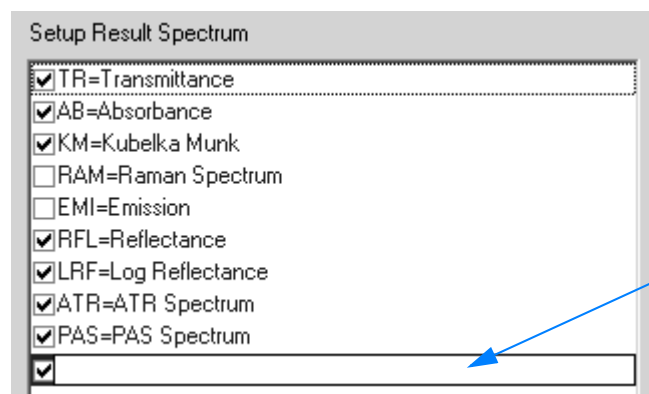
Enter the respective definition into this entry line. The entry is displayed in black. **Note: Entries displayed in black can always be edited and deleted.** To edit the entry double click into the respective entry. If a component has not yet been available (or should not be used at the moment), deactivate the respective check box.

B To move an item to a different position select it and either click on the *Item UP* or I*tem DOWN* button.

C To delete an item click on the *Delete Item* button.

D To reset the optics standard settings click on the *Restore Factory Defaults* button.

If a particular result spectrum type is not available in the list or deactivated, it cannot be selected in the measurement experiment.

> **Note: If you have created a measurement experiment and subsequently edited the optics configuration, this may cause the experiment to be incompatible to the optics settings. The ⊗ symbol appears on the *Measurement* dialog and indicates this kind of problem.**

3.11.3.3 Optic Communication

The *Optic Communication* tab allows to monitor the optics communication. Activate the *Auto Scroll* box if you want the list to automatically scroll (in case of long lists).
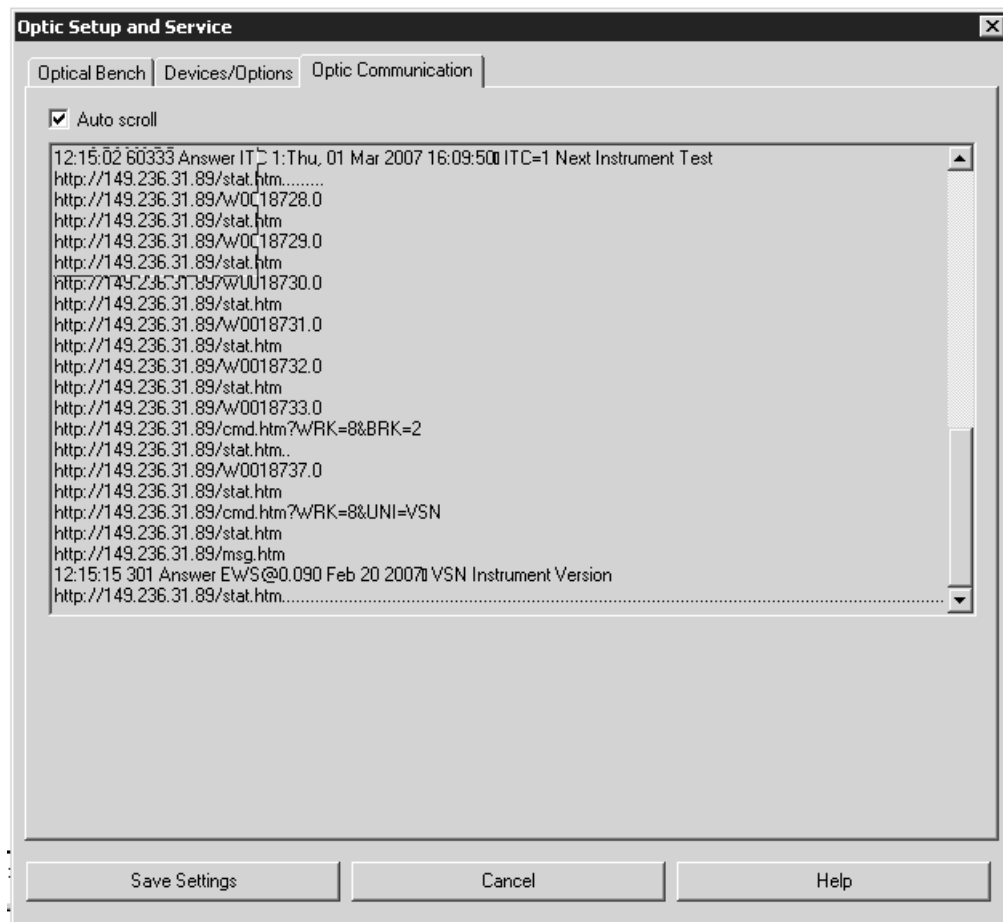
Figure 248: Optic Setup and Service - Optic Communication

3.12   Setup Menu

The *Setup* menu includes all functions to be required to configure menus and toolbars as well as the workspace.
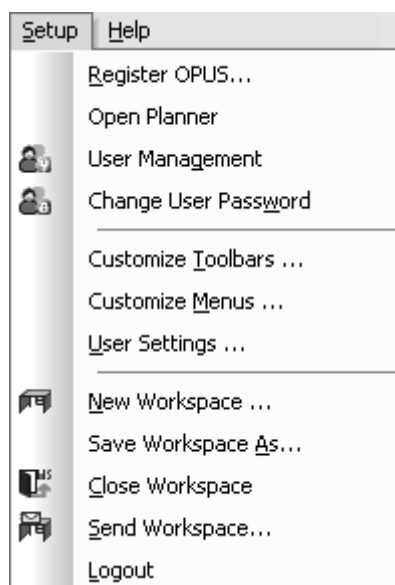
Figure 249: Setup menu

3.12.1 Register OPUS

Note: If you use OPUS in connection with an ALPHA spectrometer, no OPUS registration is required. In this case an automatic registration is done when starting OPUS for the very first time. This registration is permanently valid.

Registering OPUS is **only required** if:

- additional OPUS packages have been bought
- Bruker libraries want to be used
- the 30-days'-trial period[1] has expired

The data required (key, serial number etc.) to register OPUS in the above mentioned cases can be obtained from Bruker. The registration has to be performed only once and is valid for all users. **To be able to register OPUS you need to have Administrator rights in Windows.**

---

1. If you work without any spectrometer connected, you can use OPUS for 30 days without registering, after the program has been installed.

To register OPUS...

1   ...select the *Register OPUS* command.
2   Fill in the entry fields.
3   Confirm the settings by clicking on the OK button.

The dialog of this command is described in the following.
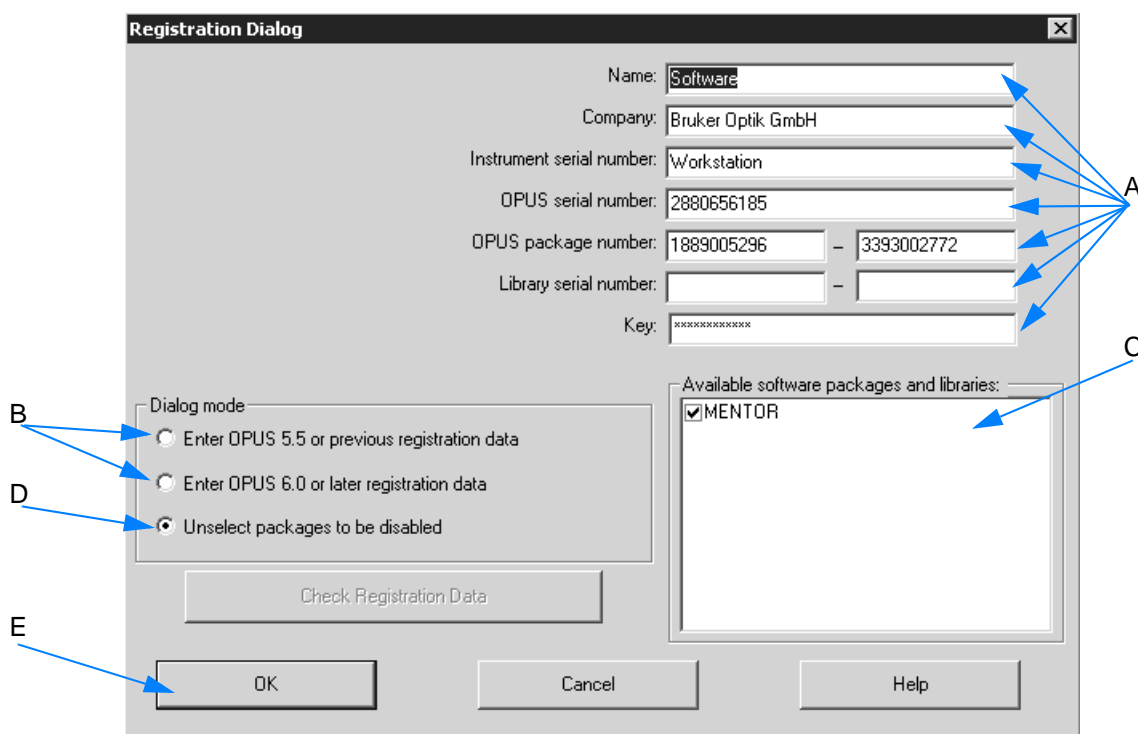
Figure 250: Registration dialog

A   Fill in the entry fields by using the data which are written on the OPUS CD for the OPUS registration. **Note: You only have to fill in those fields which you received registration data for.**

The OPUS serial, package and library number consist of figures only, whereas the key consists of both figures and capital letters. When entering the key for the first time it is displayed in plain text, later it is hidden by "*".

B   Select the option which corresponds to your OPUS version.

C   The MENTOR software package is checked by default. It is the software package available for the ALPHA spectrometer. **Do not deactivate this check box.**

D   If additional software packages have been installed, they can be deactivated by means of this option button. They will be deactivated until you restart OPUS or open the *Registration* dialog once again.

E   If you click on this button, the data are permanently registered.

3.12.2 Open Planner

Definition	The *Open Planner* command allows to exactly schedule appointments or events in a calender. Appointments are planned activities in your planner which you can also define as recurring items at a daily, weekly or monthly interval. In this context an event is an activity that lasts at least 24 hours and normally takes place once (e.g. yearly) during one day or several days.
Principle	OPUS allows to schedule the following activities: • Switching on and off the internal IR source of the spectrometer • Starting the instrument test • Activating user-specific messages Basically, the general planner setup in OPUS is similar to any other comparable planner feature based on Windows. **Note: The *Open Planner* command can only be accessed if you are entitled to change user rights and add new workspaces (see also chapter 3.12.7).**

Basic Features

If you double click anywhere on the planner, you can start defining the entry. It is also possible to colorize the entry to see at once what kind of appointment or event it is about.

When a timer item starts a message pops up and reminds you of the OPUS activity running soon.

OPUS has to run, before being able to start the scheduled item at the pre-defined time. If you select the *Open Planner* command, the following dialog opens:
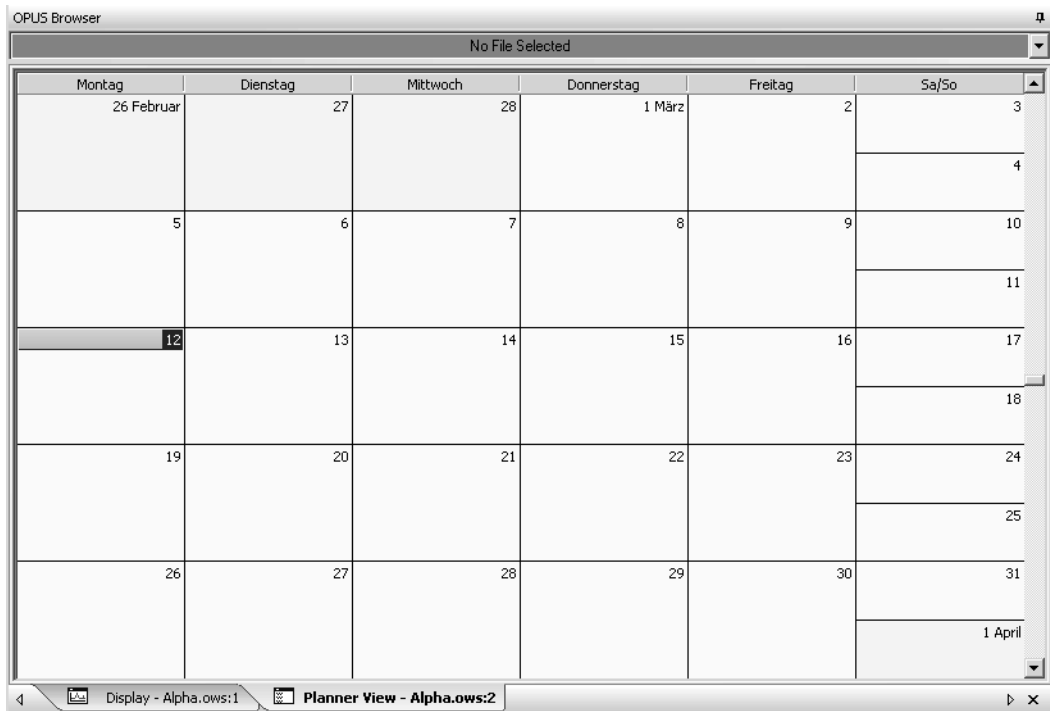
Figure 251: Planner view

3.12.2.1 View Options

OPUS provides different planner view options. By default, the month panel is displayed which you can change at any time.

To change a planner view...

1   ...right click on the panel to open the following pop-up menu:
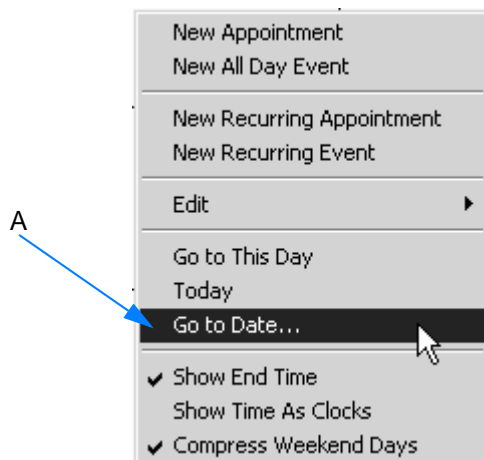
Figure 252: Planner - Pop-up menu

2   Select the *Go to Date* command from the pop-up menu. Another dialog is displayed.

A
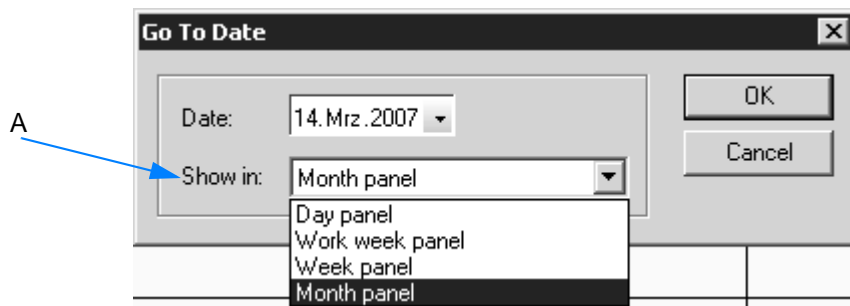
Figure 253: Planner panel selection

3   Select the desired planner panel from the *Show in* drop-down list (A in figure 253). To undo the setting made select the *Go to Date* command (A in figure 252) again and change the panel, accordingly.

Default planner view options

The following planner view options are set by default in the pop-up menu:

- Show end time: 08:00 10:00
- Compress weekend days: i.e. Saturday and Sunday are displayed in one column, one below the other

To change these default settings remove the check mark in front of the respective command in the pop-up menu (see figure 252).

3.12.2.2 Creating planner items

1   Right click on the respective day and select the *New Appointment* command from the pop-up menu.
2   Define the settings in the dialog displayed.
3   Save the settings made.

In the following the *Edit Appointment* dialog is described in more detail.

F
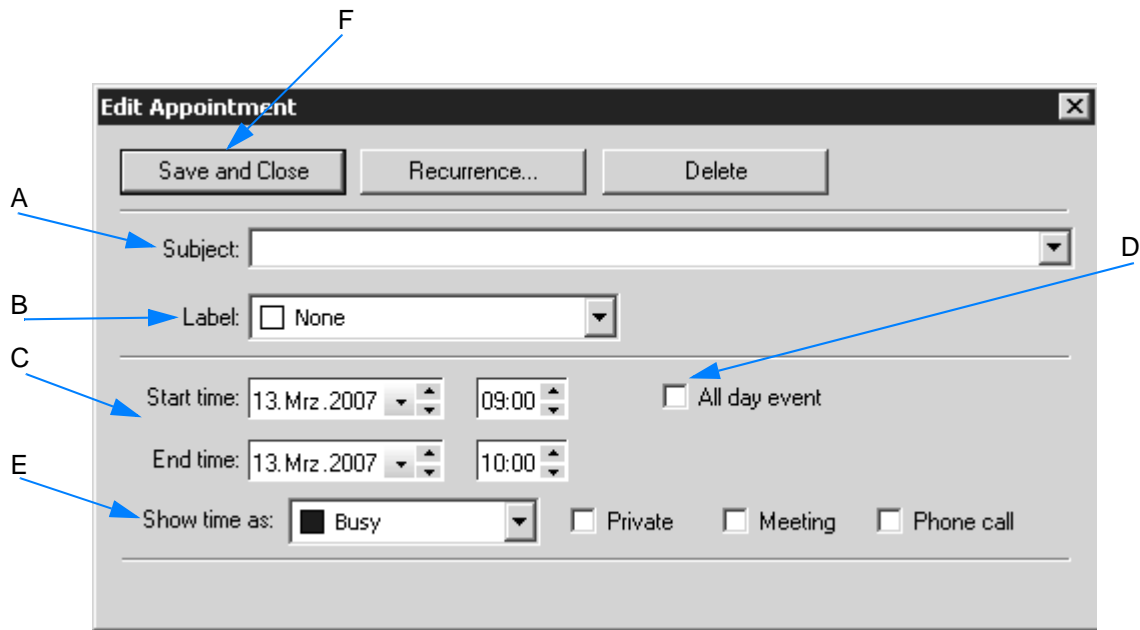
Figure 254: Edit Appointment

A   Select the OPUS activity desired from the *Subject* drop-down list. The following options are available:

- SOURCE=OFF
- SOURCE=MIR
- RUN OVP PQ TEST
- COMMAND_LINE

B   Single entries can be colorized to see at once in the planner what kind of appointment it is about. Select the color desired from the *Label* drop-down list. The entry will then be displayed by an additional color bar in the planner view.

C   Define the start and end time of an entry. Either enter the date manually into the entry field or click on the small arrow next to the entry field. In the latter case a small month panel pops up from which you can select the desired day for the respective entry.
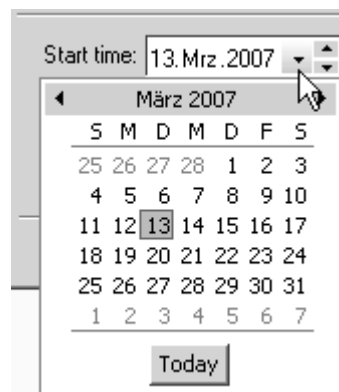
Starting from today's date you can also use the arrow keys ⏶⏷ to define the date desired. The time can be set either manually or by using the arrow keys.

D If you activate the check box, the entry becomes an event that lasts at least one day. **An all day event does not occupy blocks of time in your planner. Instead, it is displayed at the top of the date which you have specified in the planner.** This kind of event can also be created by using the *New All Day Event* from the pop-up menu (see figure 252).

E The *Show time as* drop-down list allows to define the time status of the entry. This is recommended if others have access to your planner.

F To save your settings click on the *Save and Close* button.

Note: Each single appointment or event can be changed into a recurring item, i.e. have it occurred repeatedly. In this case click on the *Recurrence* button (for details see the following chapter).

3.12.2.3 Creating recurring items

If single appointments or events are to be repeated, define these appointments or events as recurring items. A typical example of a recurring daily event is to start the instrument test at a fixed period of time, or shut down the IR source inside the spectrometer.

To create recurring items...

1 ...right click on the planner view and select the *New Recurring Appointment* or *New Recurring Event* command. The dialog that opens is the same for both commands.

2 Define the settings.

3 Confirm the settings made by clicking on the *OK* button.

4 At last, define the name of the recurring appointment or event.

In the following the *Appointment Recurrence* dialog is described.
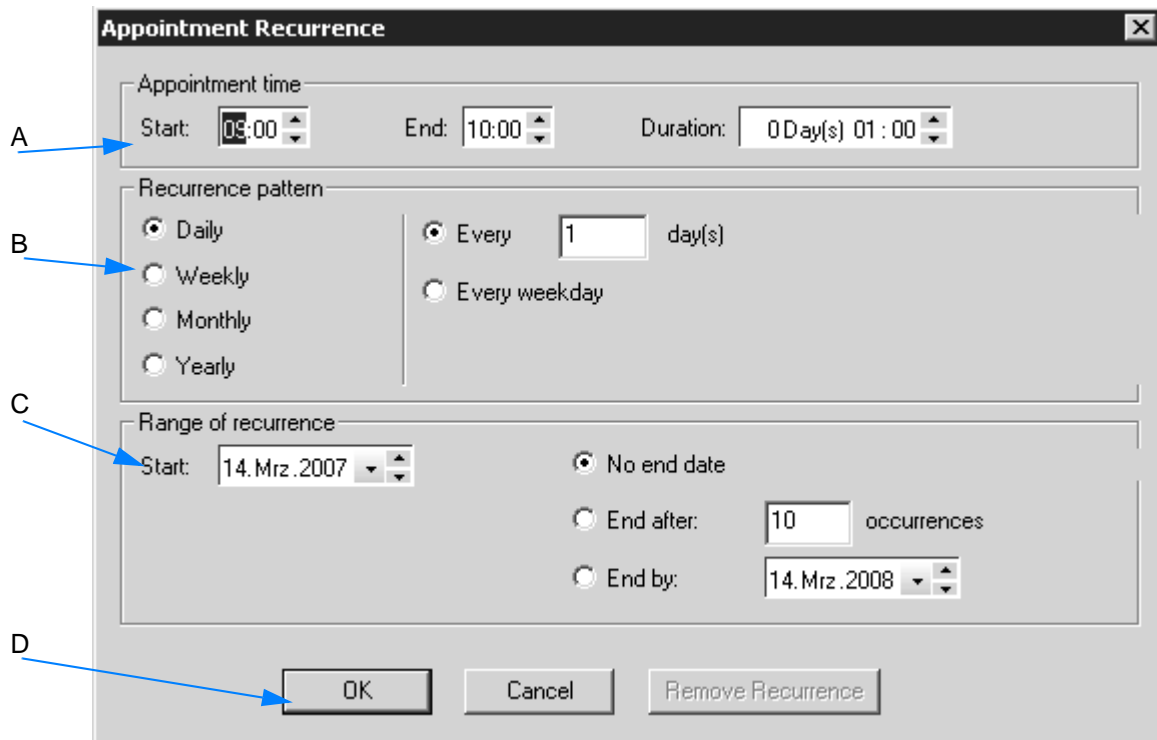
Figure 255: Appointment Recurrence

A Define the start and end time of the actual appointment or event, either manually or by means of the arrow keys.

B The recurrence pattern helps to exactly set up at what intervals the appointment or event recurrence has to take place. Activate the respective option buttons.

C The range of recurrence refers to the duration of a complete appointment or event recurrence. Define the start and end of the recurrence. Recurring items are always indicated in the planner by

the ↻ symbol.

D As soon as you confirm your settings by clicking on the *OK* button the *Edit Appointment* dialog (figure 254) is displayed. Enter the name of the recurrence into the *Subject* drop-down list, or select the corresponding activity from the *Subject* drop-down list.

3.12.2.4 Editing planner items

1 Double click on the respective entry. The *Edit Appointment* dialog (see figure 254) is displayed.

2 Make all the changes desired.

3 Save the changes made.

You can also right click on the appointment or event and select the *Open* command from the pop-up menu to have the *Edit Appointment* dialog displayed.

To rename single appointments or events in the planner...

1   ...click on the name (not on the time) of the respective entry.

2   A small white entry field opens in which you can change the current name.

| 10:30 11:00 | Test2 |
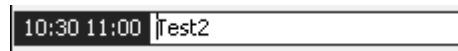
Note: To copy or delete particular entries right click on the appointment or event and select the *Copy* or *Delete* command from the pop-up menu.

3.12.2.5 Editing recurring planner items

Editing recurring appointments or events is similar to editing single appointments or events. However, a warning pops up indicating that this kind of entry selected is a recurring item.

Figure 256: Warning in case of recurring items

You can either change any aspect of a recurring appointment for the entire series, or edit a single instance of an appointment without affecting the entire series of items. Activate the corresponding option button (figure 256) and confirm the setting by clicking on the *OK* button.

The *Edit Appointment* dialog (figure 254) is displayed. If you want to change the complete recurrence pattern, click on the *Recurrence* button.

Note: Recurring items can also be copied or deleted. In the latter case a warning pops up again indicating that the entry in question is a recurring item.

3.12.3 User Management

Definition	The *User Management* command allows to create, edit or delete user records in OPUS. **This command is only available if you have OPUS administrator rights.**
Principle	To allow immediate access to OPUS a default user database is available after the installation. This default database includes three pre-defined user records, which allow full access to OPUS and all workspaces. The user records are stored in the *C:\<Program>\<OPUS>\USERDATATBASE* path in the *USERDATABASE.DAT*. The file is encrypted and cannot be modified externally. Make sure that this file is protected against accidental deletion using Windows security options. Make a backup copy whenever you modify this file, **but you must not set this file to read only.**

User Database

The pre-defined user records of the OPUS user database are as follows:

User ID	Default	Administrator	Labmanager
Password	OPUS	OPUS	OPUS
User name	Default	Administrator	Labmanager
User group	Administrator	Administrator	Labmanager
Assigned workspaces	Unlimited access to all user workspaces		

What is to be considered when creating user records?

- All entry fields which must be filled in are initially marked red. If you start typing into any of the red entry fields, the color of the entry fields changes to yellow.
- The color of the entry fields remains yellow as long as the number of characters typed in is lower than the number specified for the current field. If the minimum number of characters is reached, the entry field color changes to white indicating a valid input.

- **Double user IDs are not allowed and will be indicated by red entry fields.**
- User records cannot be stored, unless all obligatory fields have been filled in properly.

Creating User Record

Note: To be able to create user records make sure that you have OPUS administrator rights.

1   Select the *User Management* command.
2   Define the user record by means of the different tabs in the *User Management* dialog.
3   Store the settings made.

In the following the different tabs of the *User Management* dialog are described.

Setup Record
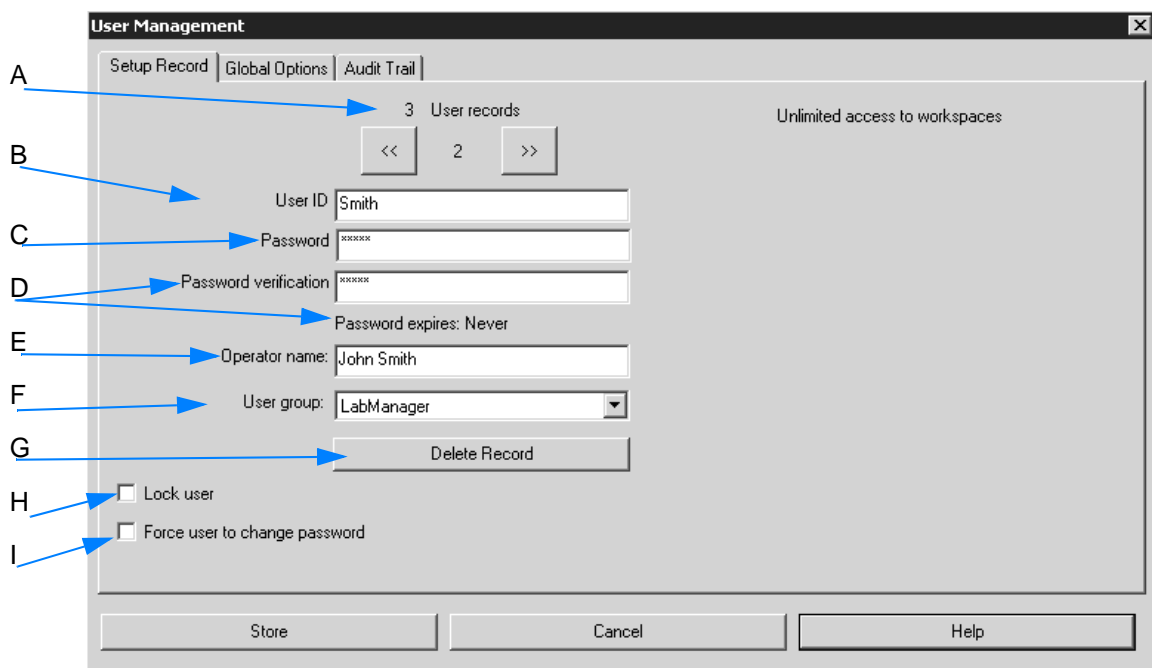
Figure 257: User Management - Setup Record

A The total number of user records is displayed in the top line of the dialog. The number of the current user record is displayed between

the ⟨⟨ and ⟩⟩ buttons. Use these buttons to go to the previous and next user records.

B Enter the user ID for the user. The user ID must have a minimum length which can be specified on the *Global Options* tab. **It is not possible to log in OPUS without any user ID.**

C Enter the password for the user. The password must have a minimum length which can be specified on the *Global Options* tab. The entry in the *Password* entry field is indicated by a number of "*". **It is not possible to log in OPUS without any password.**

D Confirm the password for verification. The entry in the *Password Verification* entry field is indicated by a number of "*".

E Enter the user name. The user name is stored in newly measured spectra and in the audit trail of spectra and methods.

F The user group specifies the access rights of a user. The drop-down list includes the *Administrator*, *Labmanager* and *Operator* user group. The first two user groups have unlimited access to all OPUS workspaces. The *Operator* user group has only access to the workspace assigned. **For users with *Operator* rights at least one workspace must be assigned.**

If you select the *Operator* user group, the list of assigned workspaces is displayed on the right.

Click on the *Add Workspace* button. Select the appropriate workspace from the dialog that opens. **OPUS workspaces are stored in the *C:\Program\<OPUS>* directory.** The name and path of the workspace selected is displayed.

To delete a workspace select it in the list and click on the *Remove Workspace* button.

G This button allows to delete the current record.

H If you activate this check box, the user will be locked. The user cannot access OPUS anymore. **This check box is automatically activated if a user tries to log in by using a wrong password several times.** The number of login attempts can be defined on the *Global Options* tab.

I   Activate this check box if you want to force the user to change his password when logging in the next time.

Global Options
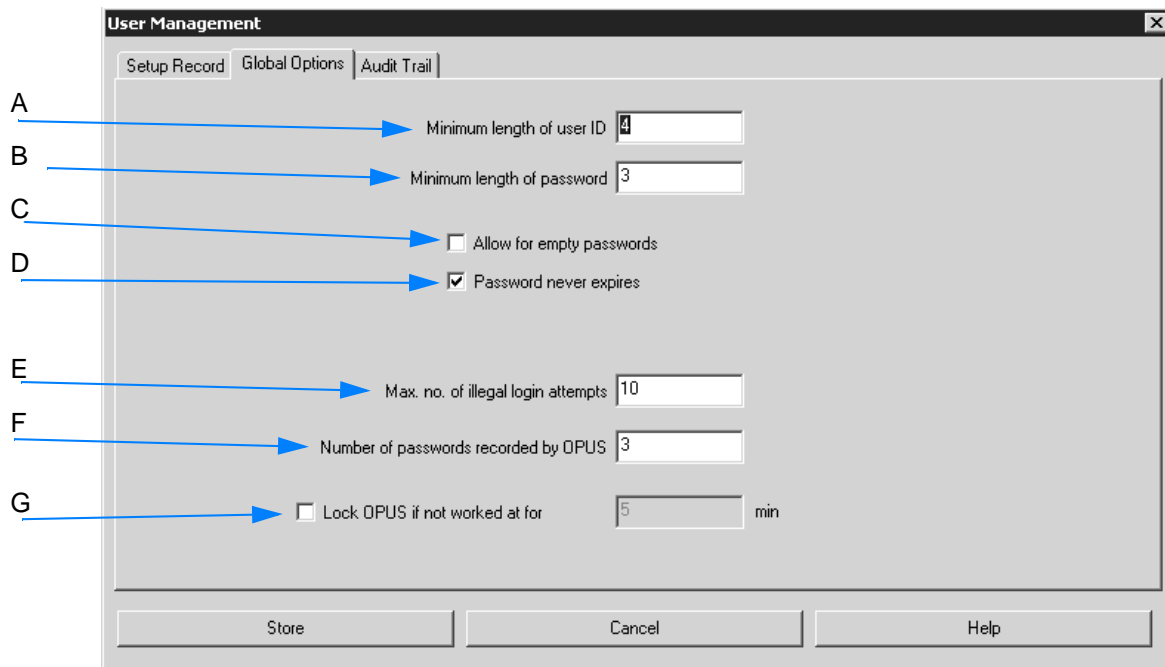
Figure 258: User Management - Global Options

A   By default, 4 characters are defined for the minimum length of the user ID. **Note that any changes made will have an immediate effect on all user records.**

B   By default, 3 characters are defined for the minimum length of the password. **Note that any changes made will have an immediate effect on all user records.**

C   If you activate this check box, empty passwords are allowed. **Note that empty passwords will never expire, regardless of the password duration set.**

D   This check box either activates or deactivates the password duration option. By default, the check box is activated. If you deactivate the check box, an additional entry field is displayed.

Define the password duration in days. **The duration period starts with the date when the user record is created or modified.**

E   In this entry field you define the maximum number of illegal login attempts. By default, 10 login attempts are defined. An illegal login is using a wrong password while trying to log into OPUS. The user

gets a warning indicating how many attempts are left. **If the last attempt has not been successful either, the user will be locked and not be able to run OPUS anymore.** Any administrator only can undo this lock by deactivating the *Lock user* check box on the *Setup Record* tab.

F　In this entry field you define the number of passwords previously used by the user, and not allowed to be used anymore when changing the password. The default setting is 3. This option forces the user to use a completely new password if the duration of his password has expired.

G　If you activate the check box, OPUS will be locked after a certain period of time has passed in which you have not worked with the PC. As soon as you have activated the check box, the entry field is enabled. Use this entry field to define the period of time in minutes.

OPUS will be locked if the defined period of time has passed. Any OPUS access will be impossible. The *OPUS Login* dialog is displayed. Note that only the previous user or an administrator can log in again. Restart OPUS to have the locking changes become effective.

Note: Any changes made on this tab have an immediate effect on all user records in the data base. Therefore, check all user records after changing any of these settings. Illegal entries will be marked in red.

Audit Trail

The *Audit Trail* tab indicates the audit trail of the following actions for each user.

- Successful login
- Login attempt of a locked user
- Login with password expired
- Changing password

For users with *Administrator* rights the following actions are additionally recorded:

- Creating or changing a user record
- Deleting user record
- Locking user record
- Unlocking user record
- Exporting audit trail
- Exporting all audit trails
- Deleting one audit trail
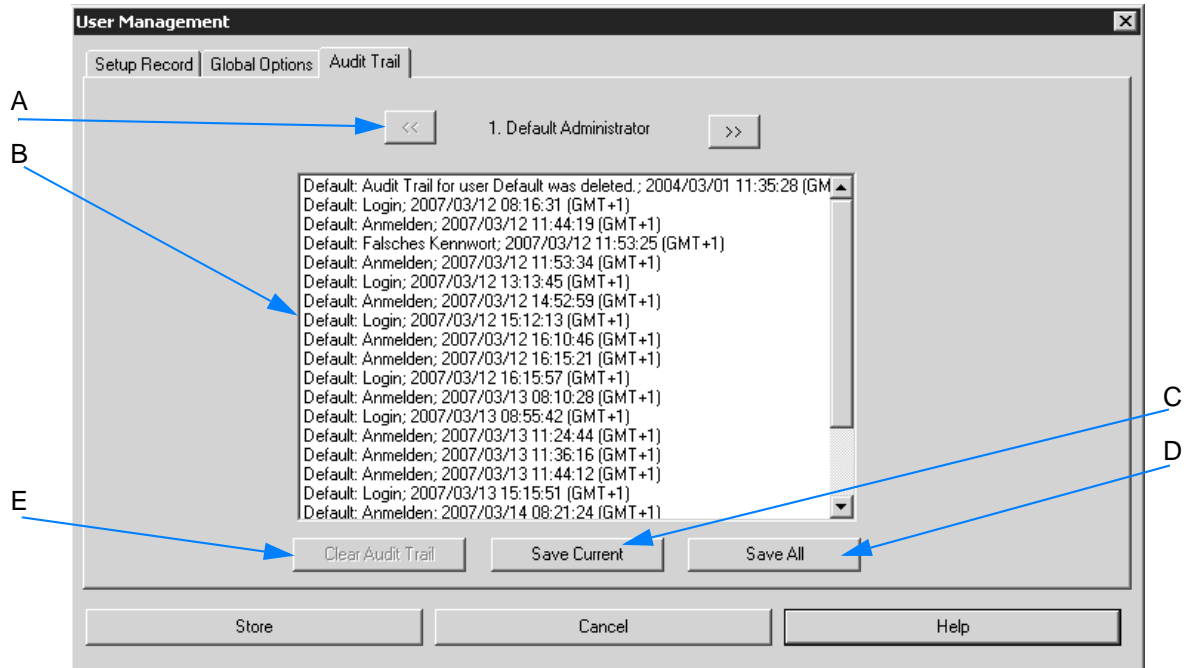
Figure 259: User Management - Audit Trail

A   Use this buttons to go to the previous or next user record.

B   This field includes the audit trail of the actions performed by the respective user.

C   Use this button to store the current user data recorded in the audit trail.

D   Use this button to store all user data recorded in the audit trail. If you click on the *Save all* button, a dialog opens. Define the file to be used to store the audit trail data and confirm the entry. Audit trail data are stored in ASCII format.

E   If you click on the *Clear Audit Trail* button, the audit trail data of the current user will be deleted. **This button is only enabled if the audit trail data have been stored first.**

Note: The *Save* and *Clear Audit Trail* actions are recorded in the audit trail of the user currently logged in.

3.12.4 Change User Password

|	
Definition	Each user can change his password. There are different reasons for changing a password: • A new user record has been created. In this case the administrator defines the initial password which will be changed by the user. • The *Password duration* option (D in figure 258) is enabled and the password has been expired according to the period of time defined. In this case the user cannot log in OPUS anymore. • The Administrator has checked the *Force user to change password* option button (I in figure 257). • A user assumes that someone else knows his password.
Principle	Select the command and specify the password changes by means of the dialog that opens. Store the changes made.
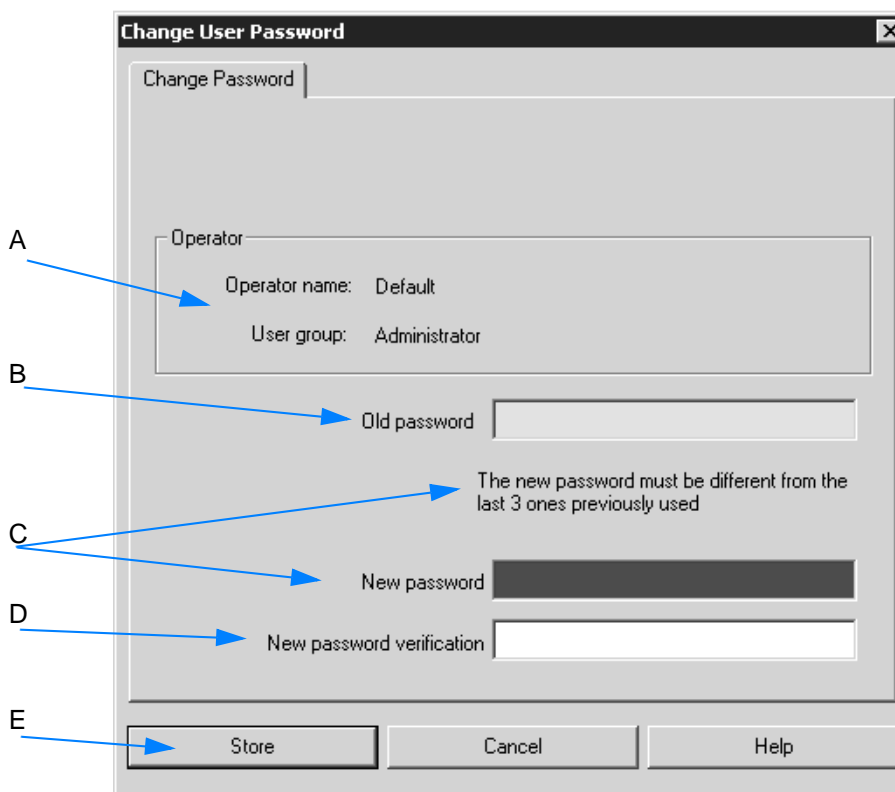
Figure 260: Change User Password

A The user name and user group are displayed.

B Enter the old password into the entry field.

C Enter the new password into the entry field. **When defining a new password make sure that it is different from the last ones previously used.** The number of passwords recorded in OPUS are

defined on the *Global Options* tab in the *User Management* dialog (F in figure 258 on page 272).

Furthermore, the new password has to have the minimum length defined on the *Global Options* tab in the *User Management* dialog (B in figure 258 on page 272).

D Enter the new password into the entry field to verify it.

E To store the changes made click on the *OK* button.

If your password has already expired...

...and you try to start OPUS, a warning pops up.

Figure 261: Warning - password expired

The *OPUS Login* dialog opens. Enter the new password and verify it.
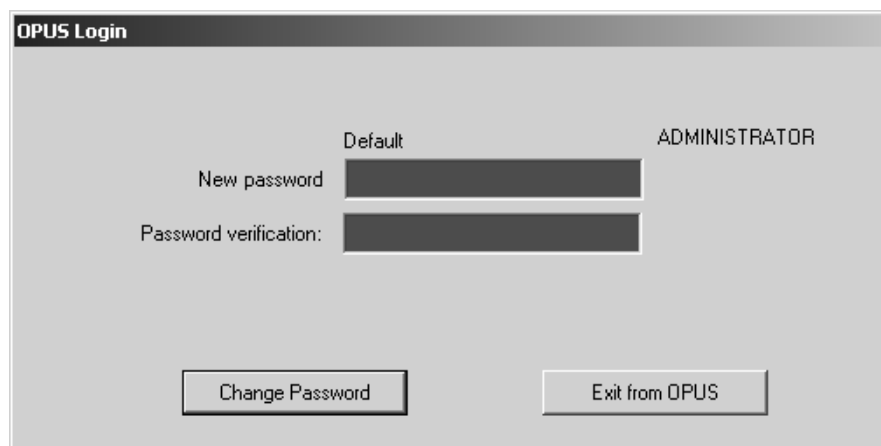

Figure 262: Enter new password

Click on the *Change Password* button. The *OPUS Login* dialog opens. You can now log in OPUS by using the new password.

3.12.5 Customize Toolbars

Definition	Customizing toolbars in OPUS is similar to any other software package based on Windows. OPUS provides the following options: • Moving toolbar • Customizing or generating toolbar • Adding, deleting or copying icons • Grouping icons on toolbar • Creating user-defined icons
Principle	There are different possibilities to modify the toolbar. These possibilities are described in the following. **In some cases it is required to have the *Customize* dialog open to be able to make changes on the toolbar.**

3.12.5.1 Moving toolbar

1   The toolbar can be freely moved. Position the cursor over the drag point ( ) at the beginning of the toolbar.

2   The cursor changes into .

3   Now, press the mouse button and move the toolbar to any position you like.

3.12.5.2 Customizing toolbar

1   Select the *Customize Toolbars* command. The *Customize* dialog opens.

2   Specify the settings.

3   The changes are immediately performed.

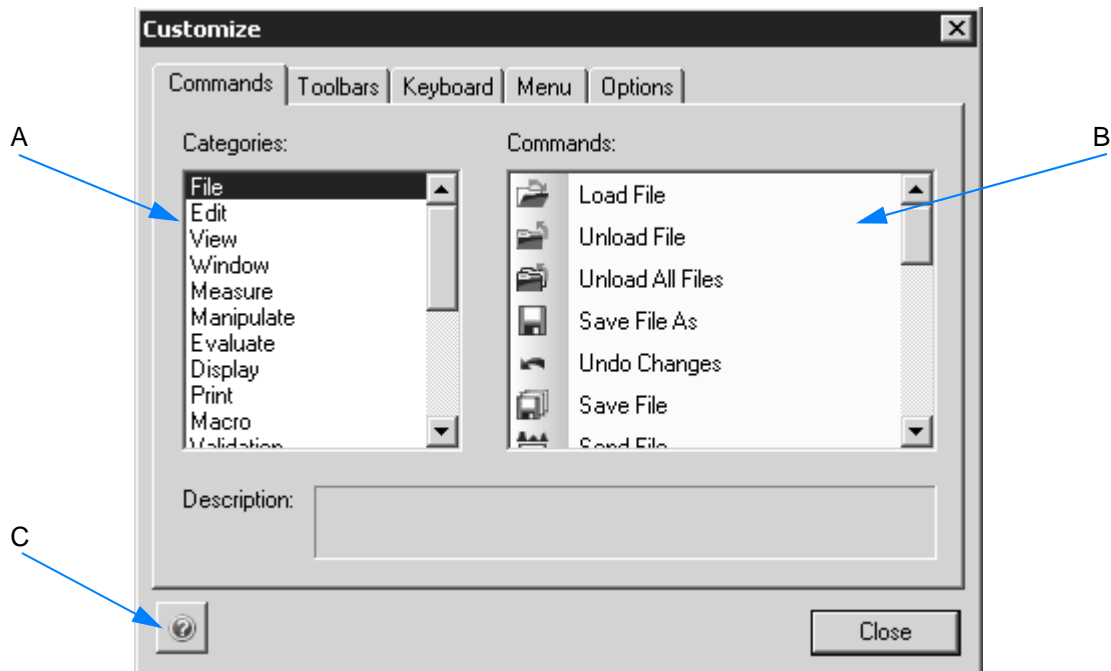The different tabs of the *Customize* dialog are described in the following.

Figure 263: Customize - Commands

A   The list box includes the different menu categories. Depending on the menu selected from the list box, all commands available for this menu are displayed in (B).

B   The list box includes the single menu commands with the appropriate icons. If you click on any command in the list box, a short text pops up describing this command.
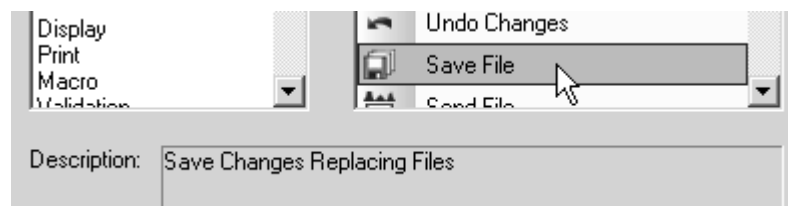
C   This button allows to open the online help of the respective tab.

To add a command to the toolbar...

1   ...click on the command in the *Command* list box (B in figure 263).

2   The cursor changes into .

3   Drag the command to the desired position in the toolbar by pressing the left mouse button.

4   If you release the mouse button, the appropriate icon of the command selected is displayed on the toolbar.

To delete a command from the toolbar

There are two possibilities:

1   Click on the appropriate icon on the toolbar and drag it from the toolbar while pressing the left mouse button. If you release the mouse button, the icon is deleted from the toolbar. **Note: Make sure that the *Customize* dialog is open.**

2   You can also right click on the icon and select the *Delete* command from the pop-up menu. **Note: Make sure that the *Customize* dialog is open, otherwise no pop-up menu will be displayed.**

To add single menus or sub-menus to the toolbar...

1   ...select the *New Menu* command from the *Categories* list box (A in figure 263).

2   Drag and drop the *New Menu* entry displayed in the *Commands* list box (B in figure 263) to the desired position in the toolbar.
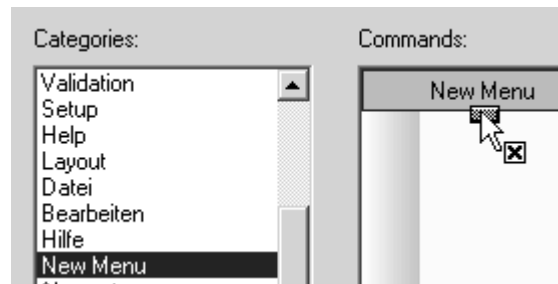
3   The new entry is displayed on the toolbar.

If you want **to change the name of the entry**, right click onto the entry and select the *Button Appearance* command from the pop-up menu. Enter the new name into the *Button text* entry field.

The new menu entry has an arrow head on the right side. Clicking on this arrow head opens a small field in which you can drag and drop single menu commands from the *Commands* list box (B in figure 263).

3.12.5.3 Creating toolbar

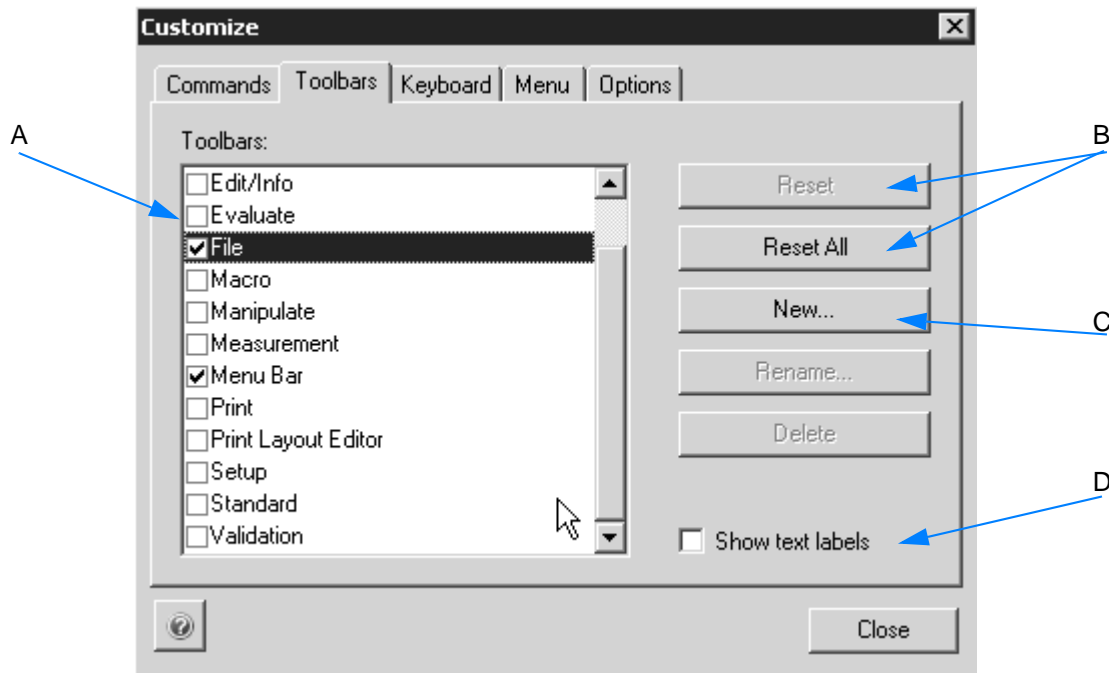Click on the *Toolbars* tab to open the following dialog:

Figure 264: Customize - Toolbars

A The *Toolbars* list box helps to define which toolbar is to be displayed on the OPUS interface. Therefore, set a check mark in front of the toolbar name. If you remove the check mark, the toolbar will be hidden.

B These buttons allow to reset the toolbar to the standard content. If you have selected several toolbars in (A), you can to reset single ones. In this case the *Reset* button will be enabled.

C This button allows to generate new toolbars.

D Toolbars can also be displayed with their text labels. Set a check mark in front of the name of the toolbar. The *Show text labels* check box is enabled. Activate this check box. The toolbar will be displayed as follows:

To create new toolbars...

1 ...click on the *New* button (B in figure 264). A dialog opens.
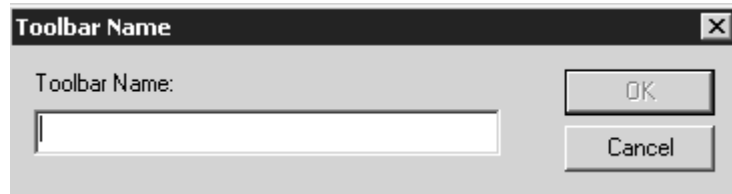
2 Enter the name of the new toolbar into the *Toolbar Name* entry field.

3 Confirm the name by clicking on the *OK* button. The new entry will be displayed on the lower end of the *Toolbars* list box (A in figure 264).

To rename or delete this new entry, select it and click on the *Rename* or *Delete* button.

Note: Toolbars which have not been created by the user cannot be deleted. If you select such a toolbar the *Reset* button will be enabled. This button allows to reset the standard icons of the toolbar.

Options tab

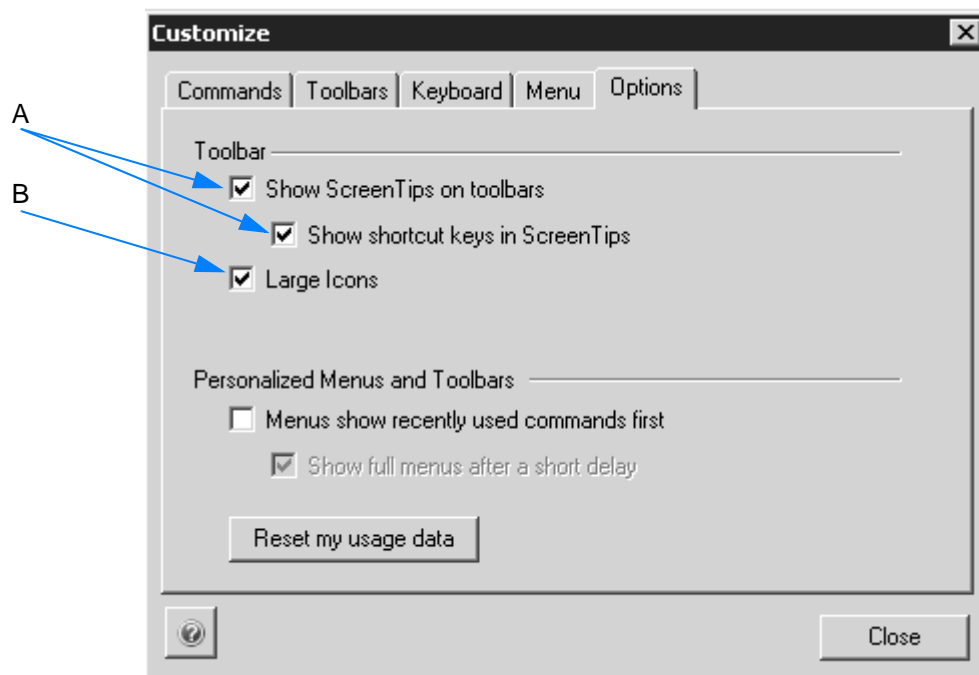Further settings on the appearance of toolbars can be made on the *Options* tab.

Figure 265: Customize - Options

A By default, the two check boxes are activated. This means that screen tips (tooltips) will be shown as soon as you move the cursor over an icon in the toolbar. The tooltip will also include the short cuts for the icon.

B By default, the check box is activated. This means that the toolbar icons will be double the normal size.

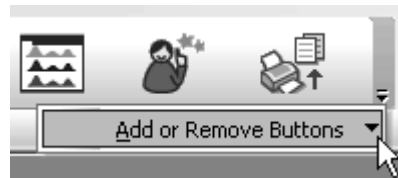For details on the menu settings in this dialog refer to chapter 3.12.6.

3.12.5.4 Adding or deleting icons

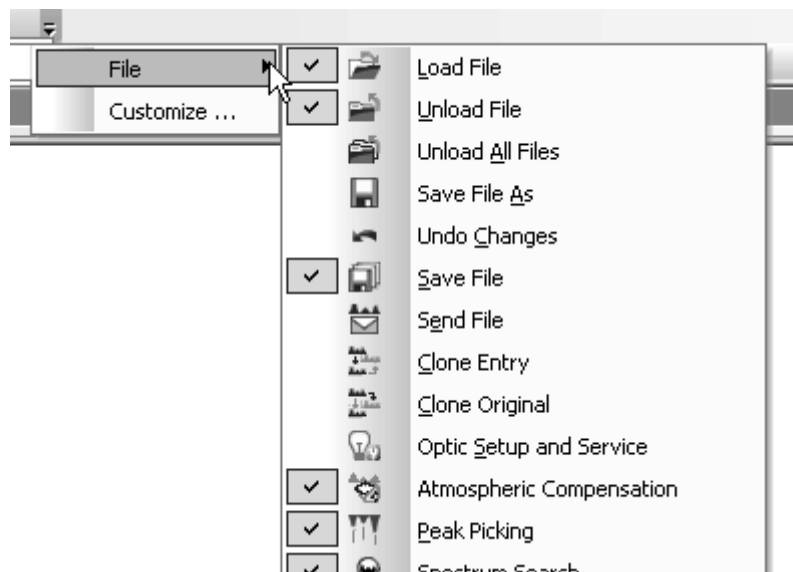1 Click on the arrow head at the end of the OPUS toolbar. An edit field pops up.
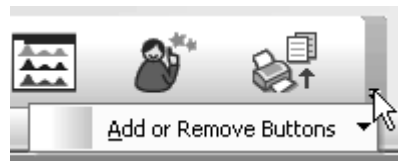
2 Position the cursor on the edit field arrow head.

3 Another edit field is displayed.

4 Position the cursor on the arrow head of the second edit field. All icons are displayed which can be added to the standard toolbar.

By default, a check mark is set in front of some icons. These icons are activated and displayed in the toolbar.

To **add** further icons to the toolbar click on the respective icon. A check mark is set in front of the icon selected. Thus, the icon is activated and displayed on the toolbar.

To **delete** an icon from the toolbar click on the check mark. The check mark is then deleted and the icon is no longer displayed in the toolbar.

3.12.5.5 Copying icons

1. Open the *Customize* dialog by means of the *Customize Toolbars* command.

2. Go to the toolbar and click on the icon to be copied.

3. Drag the icon to the desired position by pressing the *CTRL+ALT* keys on the keyboard. Otherwise, the icon will only be shifted.

3.12.5.6 Depicting icons

In general, OPUS icons can be depicted as follows in the toolbar:

- Image:

- Text:

- Image and text:

Right click on any icon in the toolbar and select the appropriate depiction type from the pop-up menu. A check mark will be set in front of the depiction type selected.
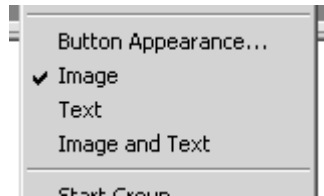
Note: Make sure that the *Customize* dialog is open. Otherwise, the pop-up menu will not be displayed.

3.12.5.7 Grouping icons on the toolbar

Icons which belong together regarding subject matter can be grouped on the toolbar. In this case you can set a dividing line in front of the first and after the last group element to differentiate between this group and the other icons and menus on the toolbar.

To add a dividing line...

1   ...right click on the desired icon while the *Customize* dialog is open.
2   Select the *Start Group* command from the pop-up menu.
3   The dividing line is added to the left side of the icon.

On a vertically positioned toolbar the dividing line is added above the icon.

To delete a dividing line between...

Right click on one of the icon and remove the check mark at the *Start Group* command in the pop-up menu.

3.12.5.8 Creating user-defined icons

1   Right click on a toolbar while the Customize dialog is open.
2   A pop-up menu is displayed.
3   Click on the *Button Appearance* command from this pop-up menu. The following dialog opens:
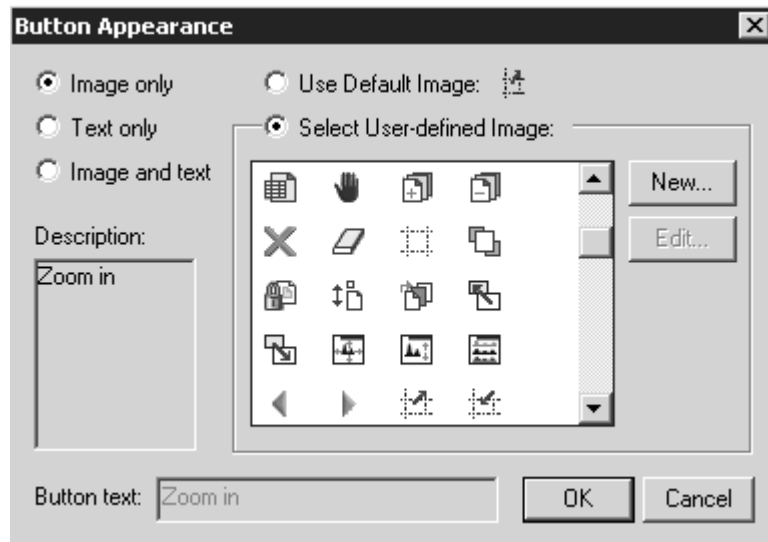
Figure 266: Button Appearance

> 4   Activate the *Select User-defined Image* option button and click on the *New* button. Another dialog opens:
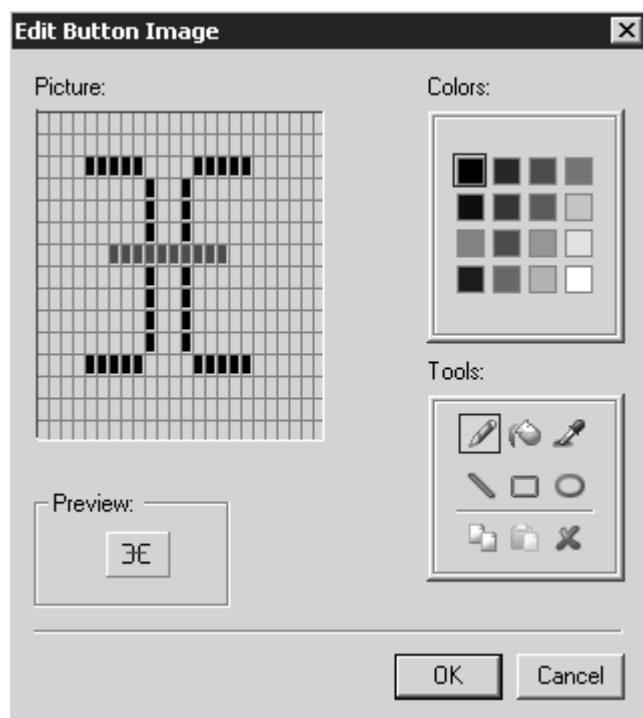

Figure 267: Edit button image

> Similar to any other drawing program a color palette and different tools are available to create your own icon. The icon drawn is displayed in the preview.
>
> To store the newly created icon click on the *OK* button. The icon will be included in the icon list box.
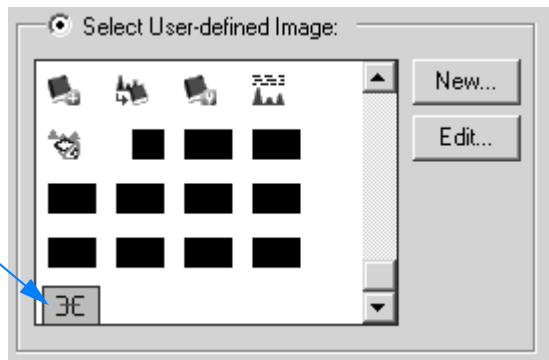
Figure 268: Newly created icon

If you want to create a name for the icon, click on the icon and activate the *Image and text* option button. The *Button* text entry field will be enabled. Now, enter an appropriate name for the icon.
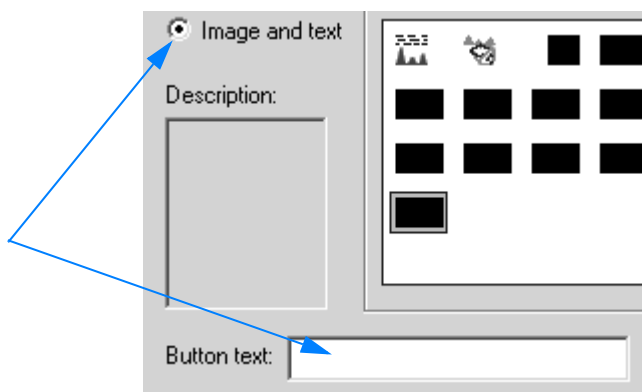
Figure 269: Create icon name

3.12.6 Customize Menus

Definition	Customizing menus in OPUS is similar to any other software package based on Windows. OPUS provides the following options: • Adding or deleting menu commands • Moving or copying menu commands • Moving or copying menus and menu commands on toolbar • Creating sub-menus • Grouping menu commands
Principle	There are different possibilities to configure the menus. These possibilities are described in the following. **To configure menus requires the *Customize* dialog to be open.**

Click on the *Customize Menus* command. In the following the *Menu* and *Options* tabs are described. The *Commands* and *Toolbars* tabs are mainly about customizing toolbars and are described in chapter 3.12.5.
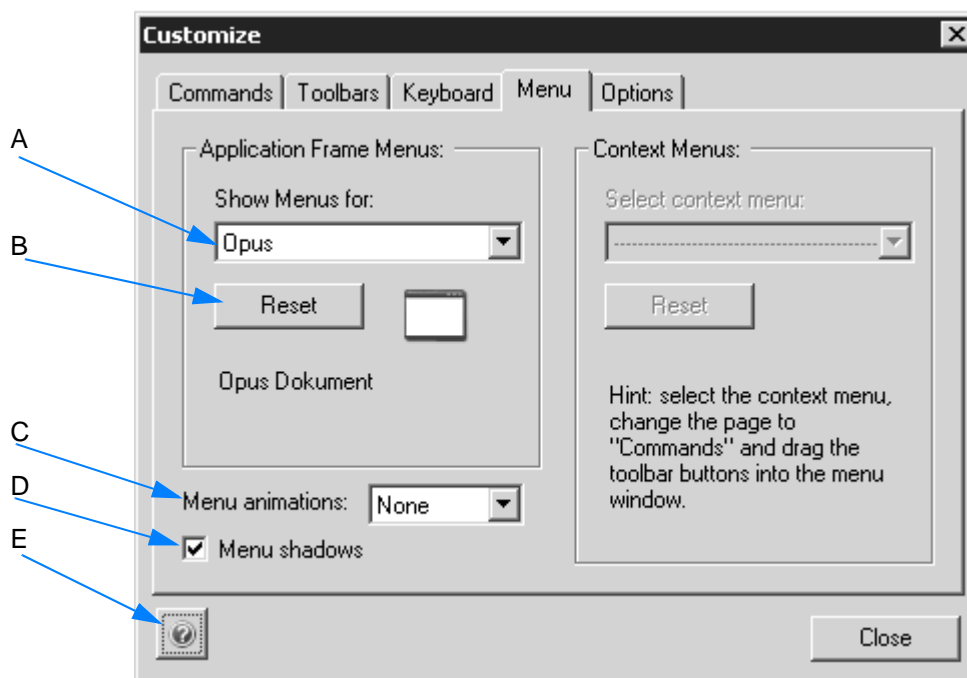

Figure 270: Customize - Menu

A Select the workspace for the menu to be customized from the drop-down list. You can edit the menus for the following OPUS work-spaces:

- OPUS
- PLE (Plot Layout Editor)
- VBScript
- GMacro
- Default Menu

B To undo the changes made click on the *Reset* button. The menus of the workspace in question are displayed again with their standard icons and commands.

C Menus can be animated. Select one type of animation from the *Menu animations* drop-down list. The following types of animations are available:

- Unfold
- Slide
- Fade

D The check box is activated by default and displays the menus with a light grey shadow on the right side.

E This button allows to open the online help of the respective tab.

Two additional general settings can be made on the *Options* **tab**. These settings have an influence on the appearance of the user-defined menus and toolbars.
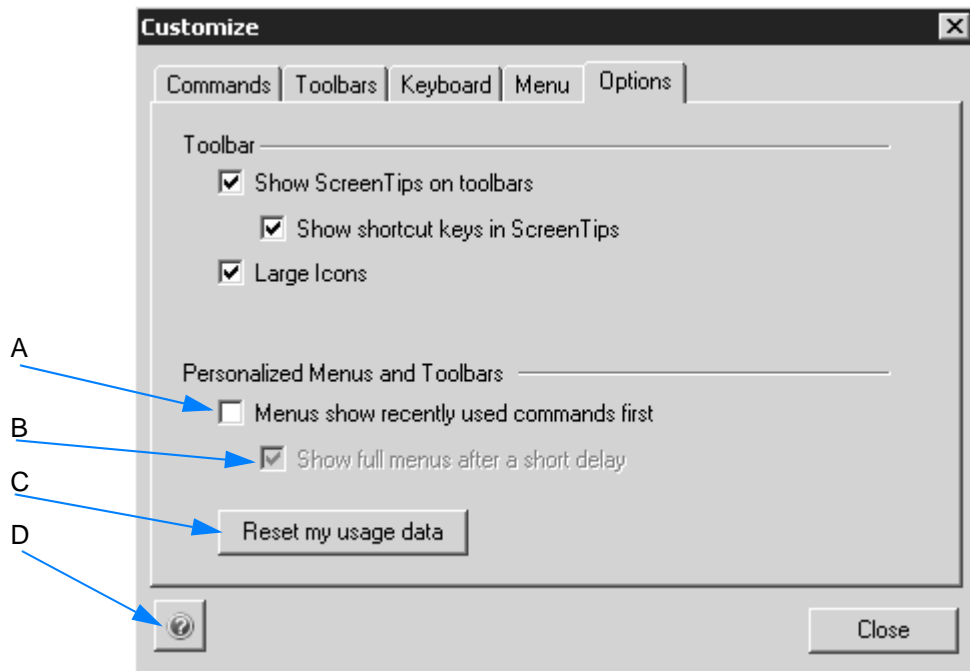

Figure 271: Customize - Options

A If you activate the check box, only those commands are displayed in the menus which have been used recently. To open the com-

plete menu view click on the double arrow (   ) below the last command shown.

B You can have the complete menu view automatically be displayed after a short period of time. Activate the check box.

C If you click on this button, all the default settings are restored.

D This button allows to open the online help of the respective tab.

Note: The settings of the customized menus are stored in the particular workspace. If you are not entitled to customize a particular workspace (also see chapter 3.12.7), the deactivated menus and commands will remain deactivated.

To have all menus and commands displayed you may have to load a different workspace.

3.12.6.1 Adding or deleting menu commands

In both cases first select the *Customize Menus* commands.

Note: Menus can only be configured, if the *Customize* dialog is open.

1 Open the menu which has to be edited.
2 Click on the *Commands* tab in the *Customize* dialog. For further information on this tab refer to chapter 3.12.5.2.
3 Use the *Categories* list box and select the menu which you want to add the command from.
4 Click on the respective command icon in the *Commands* list box.

    The cursor changes into .
5 Drag and drop the icon to the desired position in the menu you want to edit.

To **delete** a command from a menu, click on the command and remove it from the menu.

3.12.6.2 Moving or copying menu commands

In both cases click on the respective command **with the *Customize* dialog** and the menu **being open**.

Move the command to the desired position while pressing the mouse button.

To copy menu commands right click on the respective command. Press the *Ctrl+Alt* keys and drag and drop the command to the new position.

3.12.6.3 Moving or copying menus and menu commands on toolbar

Both single menu commands as well as complete menus can be moved within or copied to the toolbar. **In both cases the *Customize* dialog has to be open.**

When **moving** click on the menu or menu command and drag and drop it to the desired position in the toolbar.

When **copying** press the *Ctrl* key and drag and drop the menu command or menu to the desired position in the toolbar.

3.12.6.4 Creating sub-menus

Menu commands which belong together regarding subject matter can be sorted in sub-menus and subsumed under a main menu.

1   First, create the main menu. Click on the *Commands* tab in the *Customize* dialog

2   Select the *New Menu* command from the *Categories* list box. The *New Men*u entry is displayed in the *Commands* drop-down list.
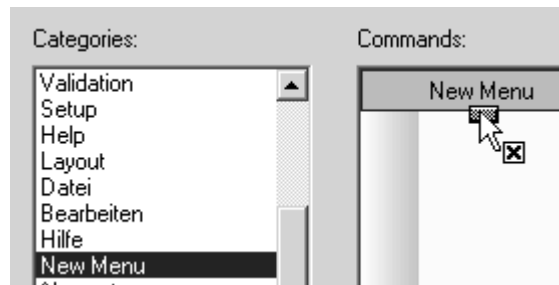
3   Open the menu which you want to edit and drag and drop the *New Menu* entry into this menu. The new entry is now displayed in the menu:

To change the name of the menu entry...

1   ...right click on the menu entry.

2   Select the *Button Appearance* command from the pop-up menu. The following dialog opens:
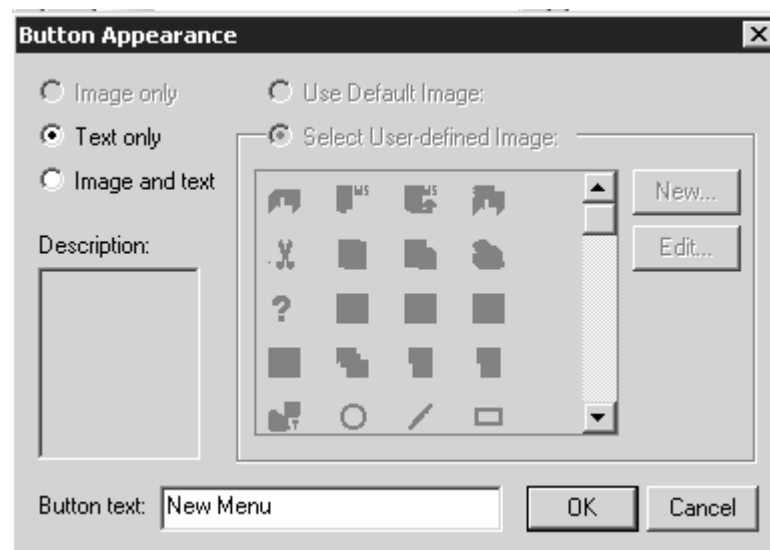

Figure 272: Change name of menu entry

3   Define an appropriate name for the new menu entry in the *Button text* entry field. Click on the *OK* button.

The new menu entry has a small arrow head on the right side. If you click on this arrow head, a small field opens in which you can drag and drop the sub-menu commands.

Select the respective command with the appropriate icon either from the *Commands* list box in the *Customized* dialog or from the menu itself. Drag and drop this command into the small entry field next to the arrow head.

Figure 273:　Example of a main menu command with sub-menus

3.12.6.5 Grouping menu commands

Menu commands which belong together can be grouped within a particular menu, i.e. in front of the first and after the last element of a group you can add a dividing line. This allows to distinguish the group from other commands within a specific menu.

To add a dividing line...

1　...right click on the menu command **with the *Customize* dialog being open**.
2　Select the *Start Group* command from the pop-up menu.
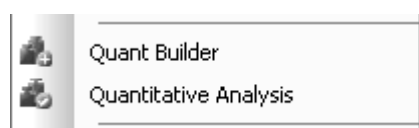3　The dividing line is set above the menu command selected.

Figure 274:　Example of grouping menu commands

To delete a dividing line...

1　...right click on the respective command.
2　Remove the check mark in front of the *Sort Group* command from the pop-up menu.

3.12.7 User Settings

Definition	OPUS user accounts can be created and managed by means of the *User Settings* command. Make sure that you have the necessary user rights to do so (see figure 276).
Principle	Select the command. Define the user settings by means of the different tabs from the dialog that opens. To confirm the settings click on the *OK* button.

The different tabs of the *User Settings* dialog are described in the following.
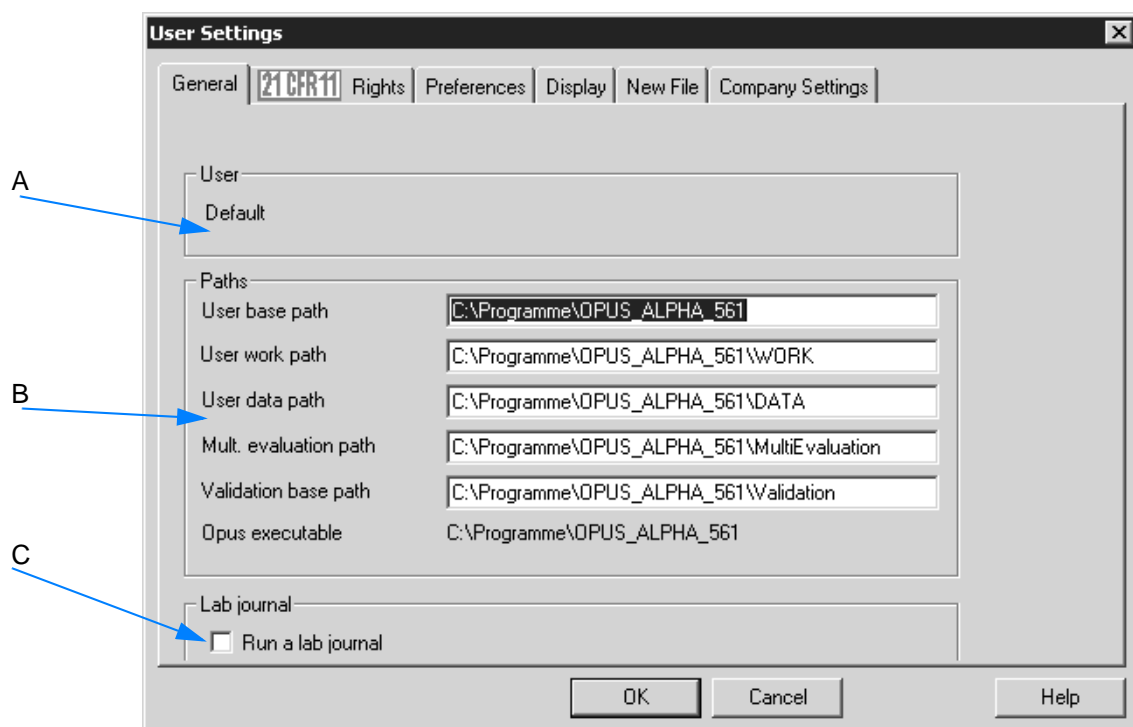

Figure 275: User Settings - General

A The user status is indicated.

B The paths for the OPUS system directories are displayed.

C If a lab journal is to be created in OPUS, the check box has to be activated. For details on the lab journal refer to chapter 3.1.8.

21CFR11 Rights

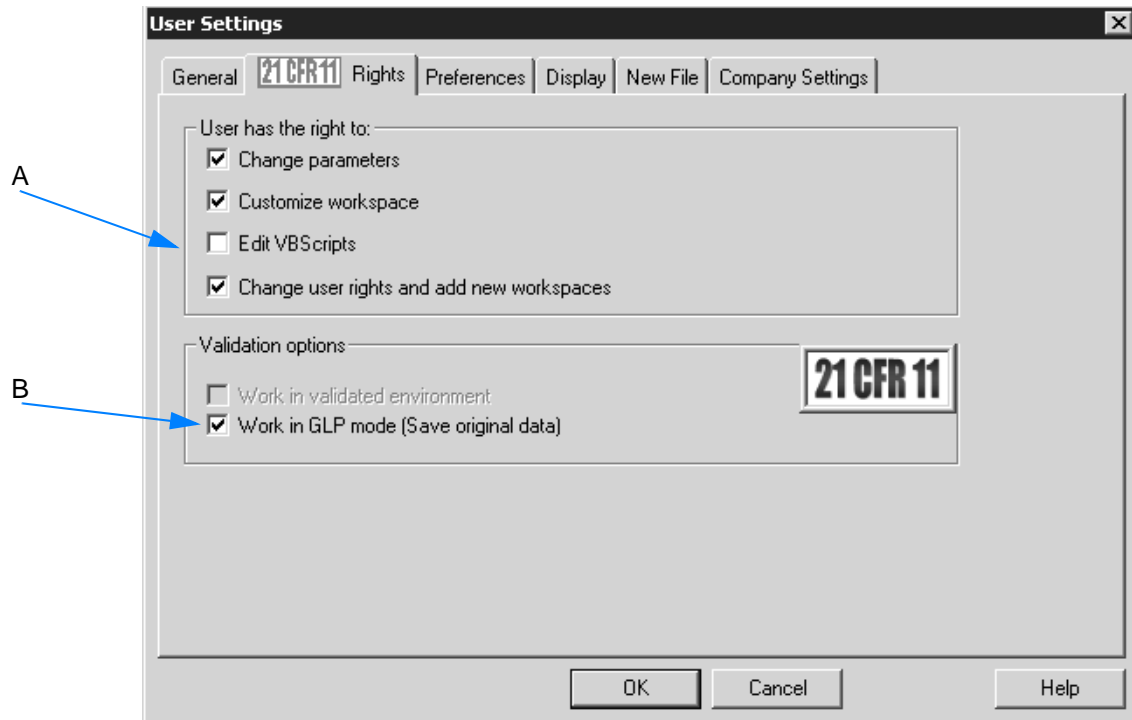Figure 276: User Settings - 21CFR11 Rights

A Define the specific rights for the user account. Activate or deactivate the corresponding check box. **Make sure that at least one administrator account includes all the user rights which can be assigned to.**

B If you activate the check box, you work in GLP[1] (Good Laboratory Practice) mode.

---

1. GLP means Good Laboratory Practice and is some kind of quality assurance directive.
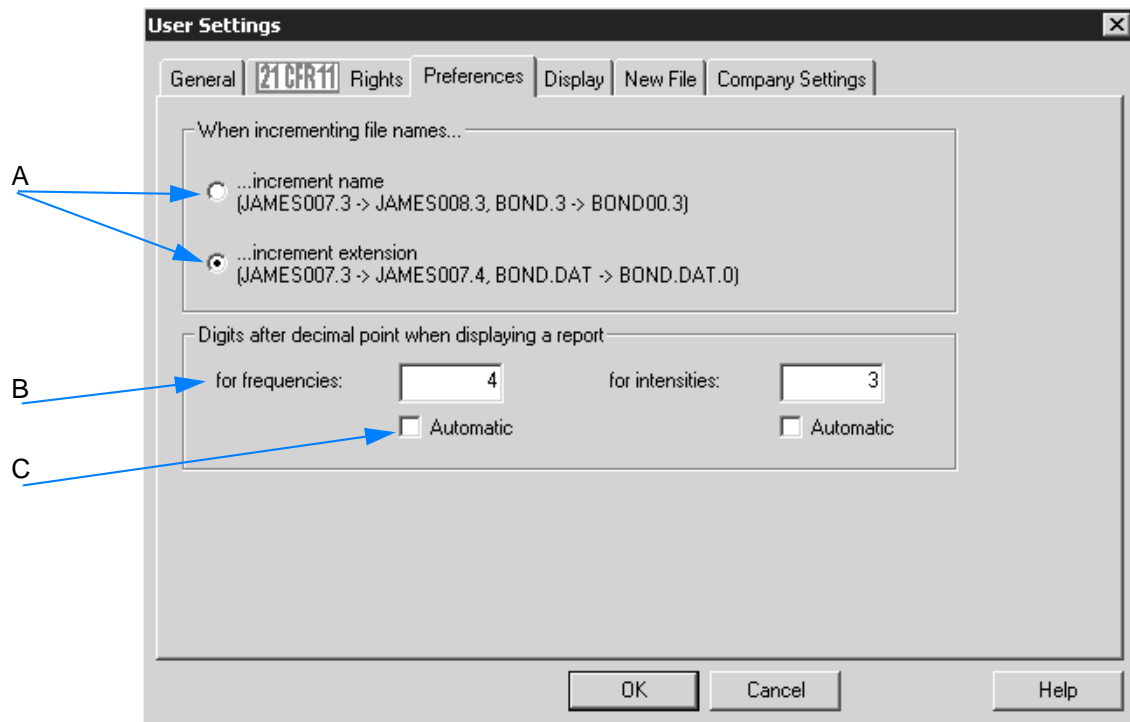
Preferences

Figure 277: User Settings - Preferences

A Define how to proceed in OPUS if you want to save a measurement by using an already existing file name. Check the respective option button.

B The default decimals for frequencies are 4 and for intensities 3. The number of decimals are displayed in the report view.

C If you want to have the number of decimals automatically set, activate the *Automatic* check box for both frequencies and intensities.
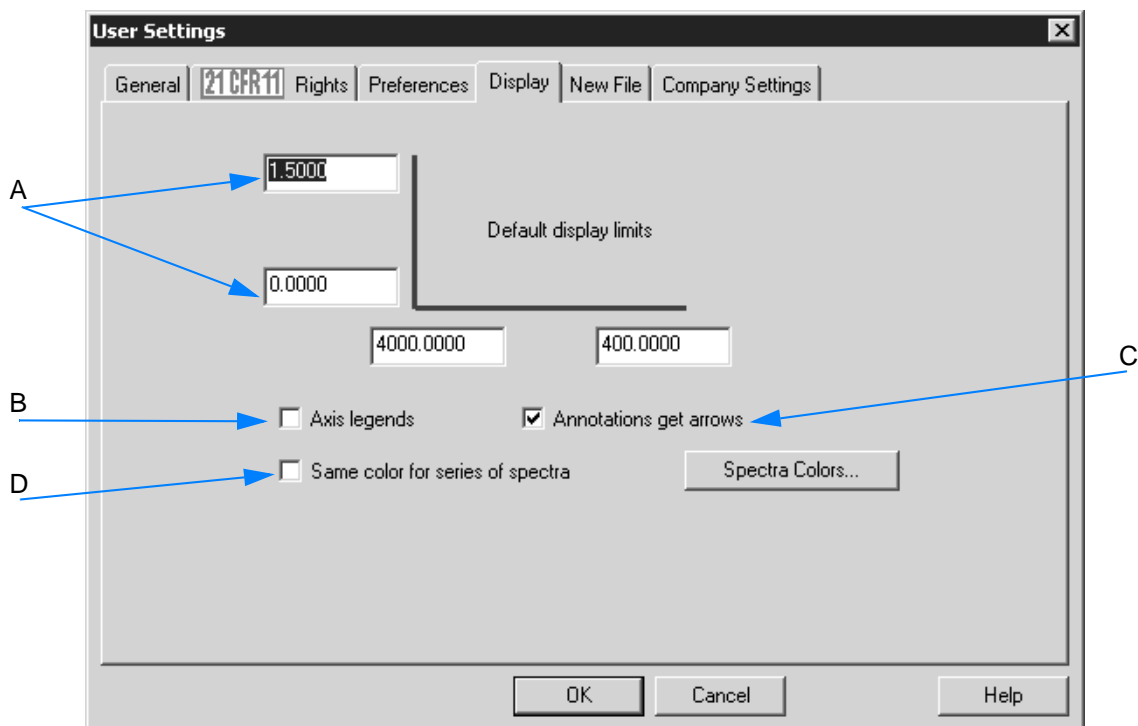
Display

Figure 278: User Settings - Display

    A The display limits are set by default. To change the limits enter the appropriate figures into the entry fields.

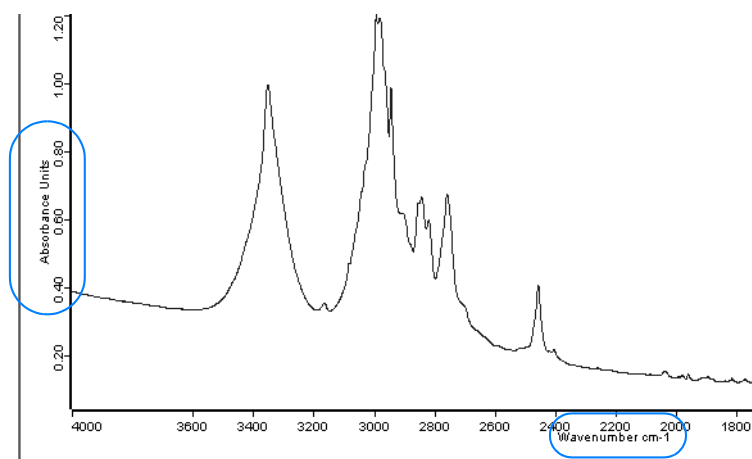   B If you activate the check mark, define whether the axes should have legends.

Figure 279: Spectrum display with axis legend

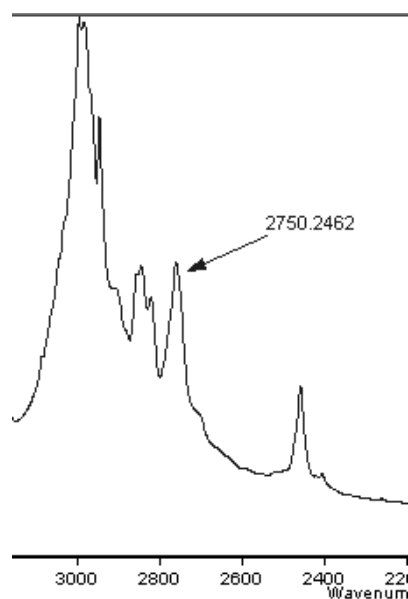C Annotations (wavenumber by default) to a spectra are displayed with an arrow. See also chapter 1.13.1.

Figure 280: Spectrum with annotation

If you deactivate the check box, the annotation will have no arrow.

D The check box allows to display spectra, which have the same basic file name, in one specific color during a particular loading procedure. **Usually, the spectral curve colors are automatically assigned when loading spectra into the OPUS browser window.**

If you activate the check box, two additional option buttons will be displayed.

If you activate the *Whole file name* option button, all spectra with the same file name (without extension) will be displayed in the same color.

Activate the *File* name check box if only a specific number of file name characters has to be identical. **Example:** if a file name has 12 characters and you enter 1 into the *First character* entry field and 8 into the *Length* entry field, the first 8 characters of any file name will be checked to see whether they are conform with the file name series.

Click on the *Spectra Colors...* button to assign a color sequence to the spectra. The following dialog opens:
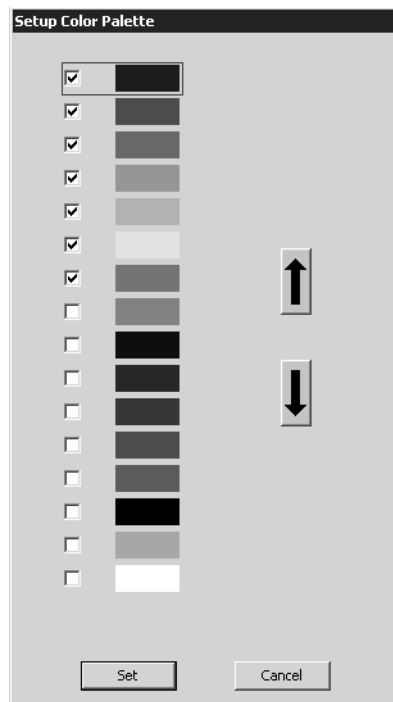
Figure 281: Setup Color Palette

The standard range of colors include 16 colors defined by default, whereby only those colors checked will be assigned to spectra.

If you have checked a color, use the arrow buttons to move it to the appropriate position, either upwards or downwards. **The color sequence defined on the color palette correlates with the spectra color displayed in the spectrum window. Therefore, the first color on the color palette corresponds to the color of the first spectrum displayed, the second color corresponds to the color of the second spectrum and so forth.** To save the settings click on the *Set* button.
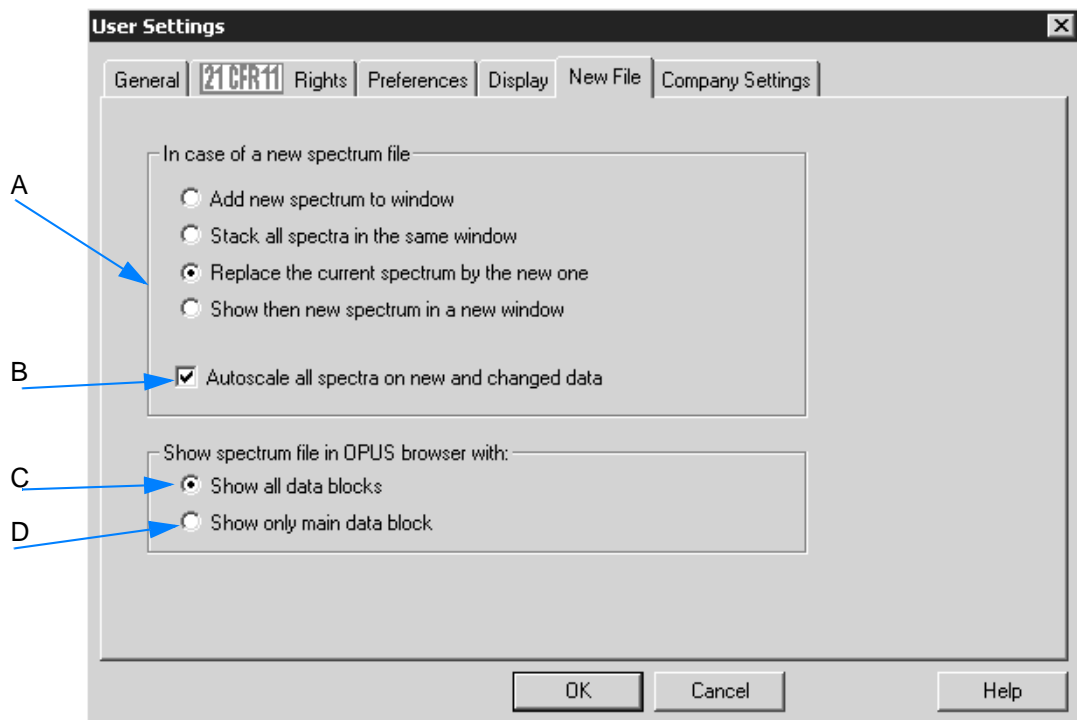
New File

Figure 282: User Settings - New File

A Define how a new spectrum file loaded or measured is to be integrated into the spectrum window. Activate the respective option button. By default, a new spectrum file loaded replaces the current spectrum displayed in the spectrum window. This means, if a spectrum has already been displayed in the spectrum window it will be removed.

B This check box is activated by default. All spectra will automatically be autoscaled.

C This option button is activated by default. All data blocks are shown in the browser.

D If you activate this option button, the main data blocks only (i.e. spectra data blocks) will be shown in the browser. In this case highbrowism will not show data blocks generated after manipulation or evaluation procedures.
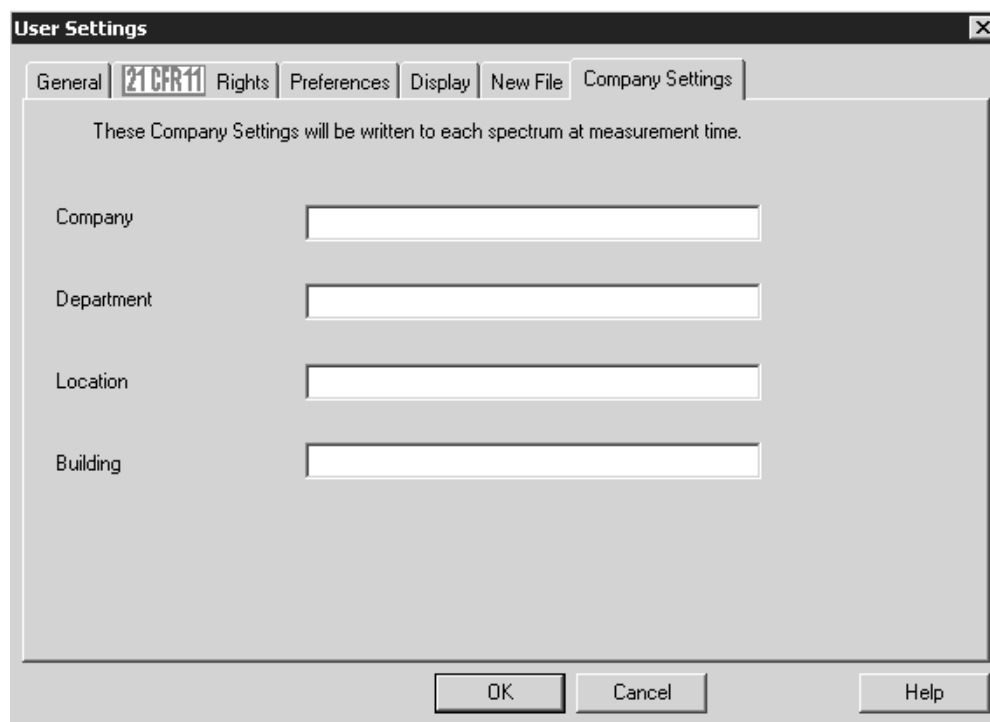
Company Settings

Figure 283: User Settings - Company Settings

On the *Company Settings* tab you can optionally define standard data for different company features. Once these entries have been defined they will be written in each OPUS file when a measurement is performed.

3.12.8 New Workspace

Definition	This command allows to create a new workspace, and is only available if the user has the right to do so (see chapter 3.12.7).
Principle	The following settings are stored in an OPUS workspace: • All user rights • Configuration of toolbar and windows • Parameters (settings) of all commands • Configuration of menus and pop-up menu

If you have selected this command, a copy of the workspace recently used will be created. At the same time the *User Settings* dialog opens. This dialog allows to define important workspace settings (see chapter 3.12.7). Save the workspace by using the *Save Workspace As* command (see chapter 3.12.9).

3.12.9 Save Workspace As

Definition	This command allows to store the workspace by using a specific name. **By default, workspaces are stored in the *C:<Program>\<OPUS>* directory.**
Principle	If you have **changed** a workspace, e.g. by re-positioning toolbars, this modified workspace will automatically be stored when you exit OPUS. If you have **created** a **new** workspace, a dialog pops up requesting the name of this new workspace when you exit OPUS.

3.12.10 Close Workspace

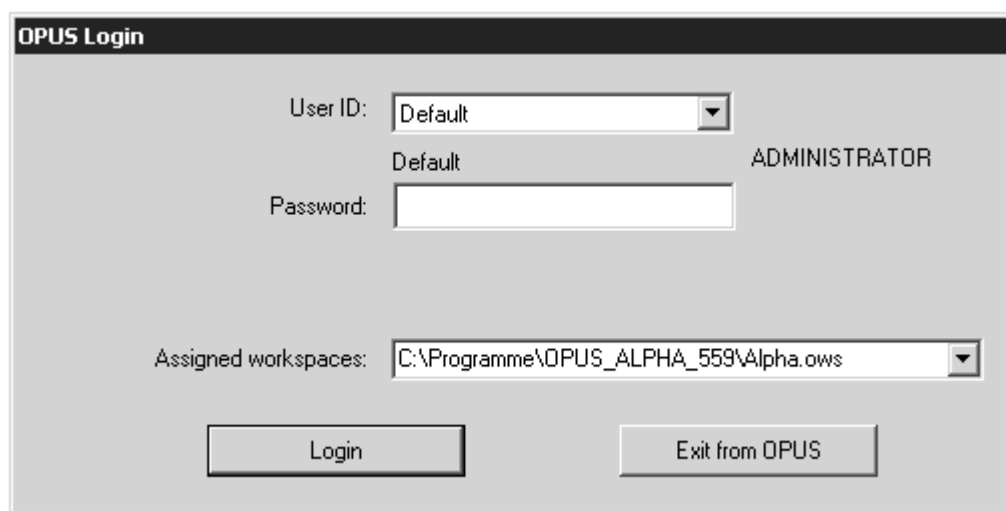|	
Definition	This command allows to close the current workspace.
Principle	This command forces to unload all files, and stop all processes running.

3.12.11 Send Workspace

Definition	This command allows to send the OPUS workspace by e-mail. In this case the e-mail addressee accepts all OPUS settings valid on your computer. The addressee has to store the OPUS workspace file on his computer, and open the file by OPUS.
Principle	Make sure that each path correlate to the OPUS settings. Therefore, sending workspaces does only make sense if the computer configuration with regard to the installation paths is identical.

3.12.12 Logout

Definition	This command allows to log out the current user and login a new one.
Principle	If you select this command, the *Login* dialog is displayed (see chapter 1.3). • Select the correct user ID from the drop-down list. The user last logged in will be displayed by default. • Enter the correct user password. • Select one of the workspaces using the drop-down list. • Click on the *Login* button to log in the new user. If you click on the *Exit from OPUS* button you close the login dialog and terminate OPUS.

Note: The *Logout* command does not unload files from the browser, nor stops processes still running (e.g. measuring).

Figure 284: OPUS Login

3.13   Help Menu

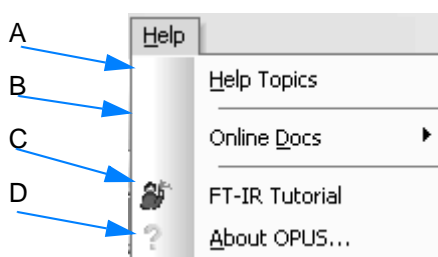

Figure 285: Help menu

A If you click on this command, the OPUS online help starts. The online help can also be started by the F1 key on the PC keyboard. **To be able to use the online help function you have to install Microsoft Internet Explorer 5.0 (or higher).**

B If you position the cursor on this command, the names of the online manuals available in OPUS are indicated. The online manuals are are provided as PDF files. **In order to read these PDF files you have to install the Acrobat Reader from the OPUS CD.**

C The FT-IR Tutorial imparts basic knowledge about FT-IR spectroscopy.

D Click on the command to learn something about the OPUS version used, the registered user name and the OPUS software package available (see also chapter 1.3).